Elevating nanoHUB to the Next Level

Assessment

Funding renewed for next 5+5 years

Past first annual review

Nathan Denny
Dwight McKay
Swaroop Shivarajapura
Steven Snyder

Michael Zentner

Purdue University, Information Technology at Purdue

nanoHUB.org usage 2013-02-01 00:00:00

ON SAFARI IN NANOHUB

THE HUNT FOR PROTOTYPICAL USERS

ON SAFARI IN NANOHUB

Motion in Time

THE HUNT FOR PROTOTYPICAL USERS

ON SAFARI IN NANOHUB

Motion in Time

THE HUNT FOR PROTOTYPICAL USERS

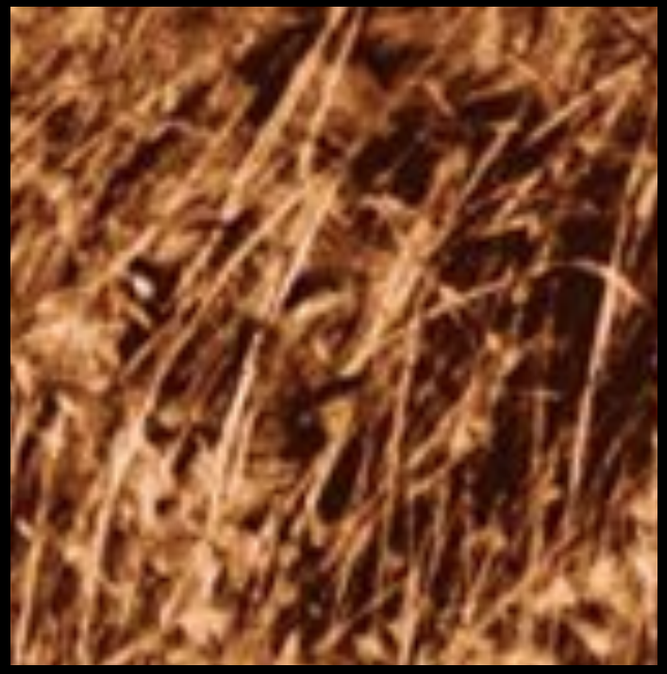
ON SAFARI IN NANOHUB

Motion in Time

THE HUNT FOR PROTOTYPICAL USERS

ON SAFARI IN NANOHUB

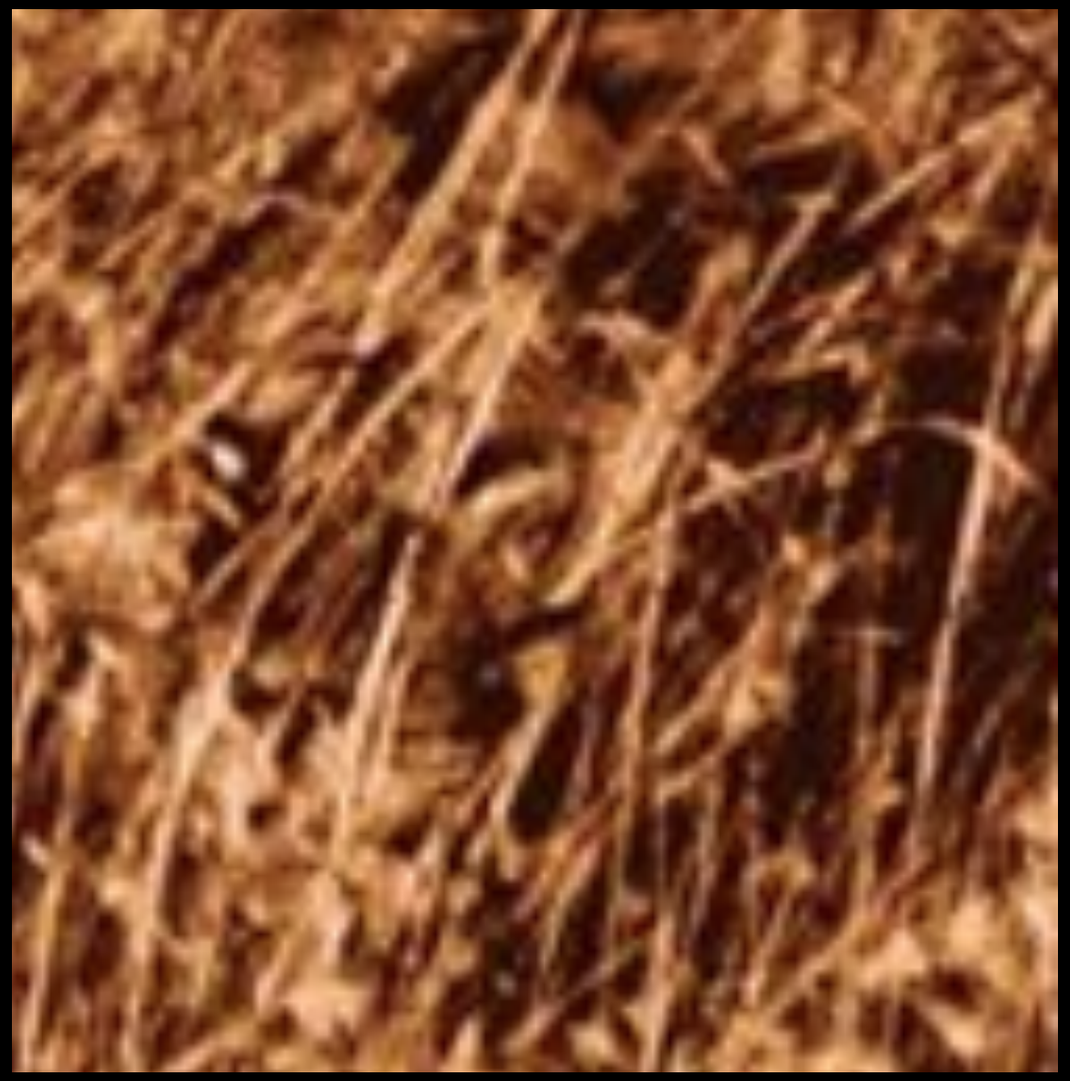
Selection



THE HUNT FOR PROTOTYPICAL USERS

ON SAFARI IN NANOHUB

Selection



THE HUNT FOR PROTOTYPICAL USERS

ON SAFARI IN NANOHUB

Filtration

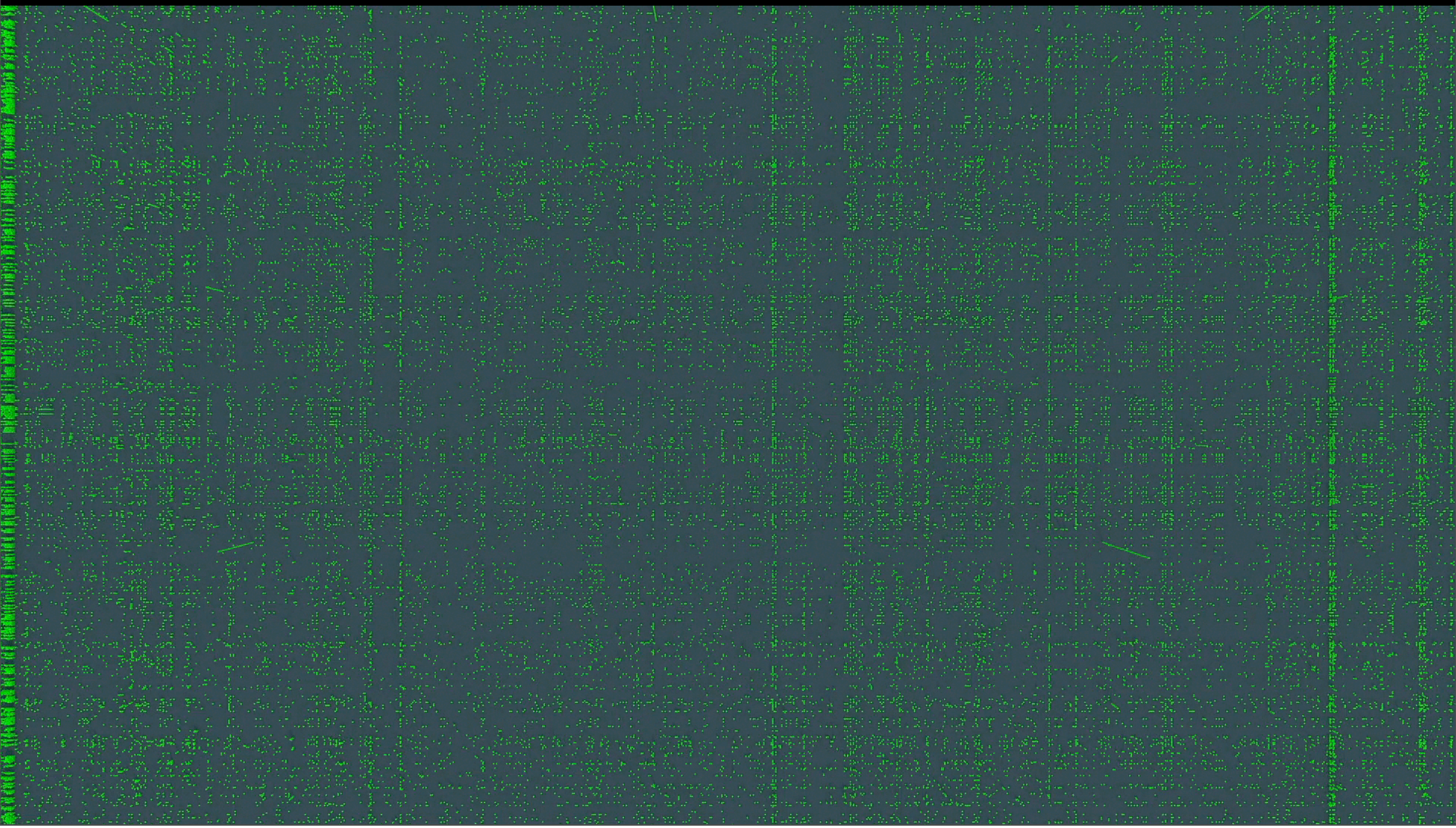
THE HUNT FOR PROTOTYPICAL USERS

Examples

nanoHUB Is Its Own Savannah

Examples

nanoHUB Is Its Own Savannah



3 Ongoing Hunts

Completeness

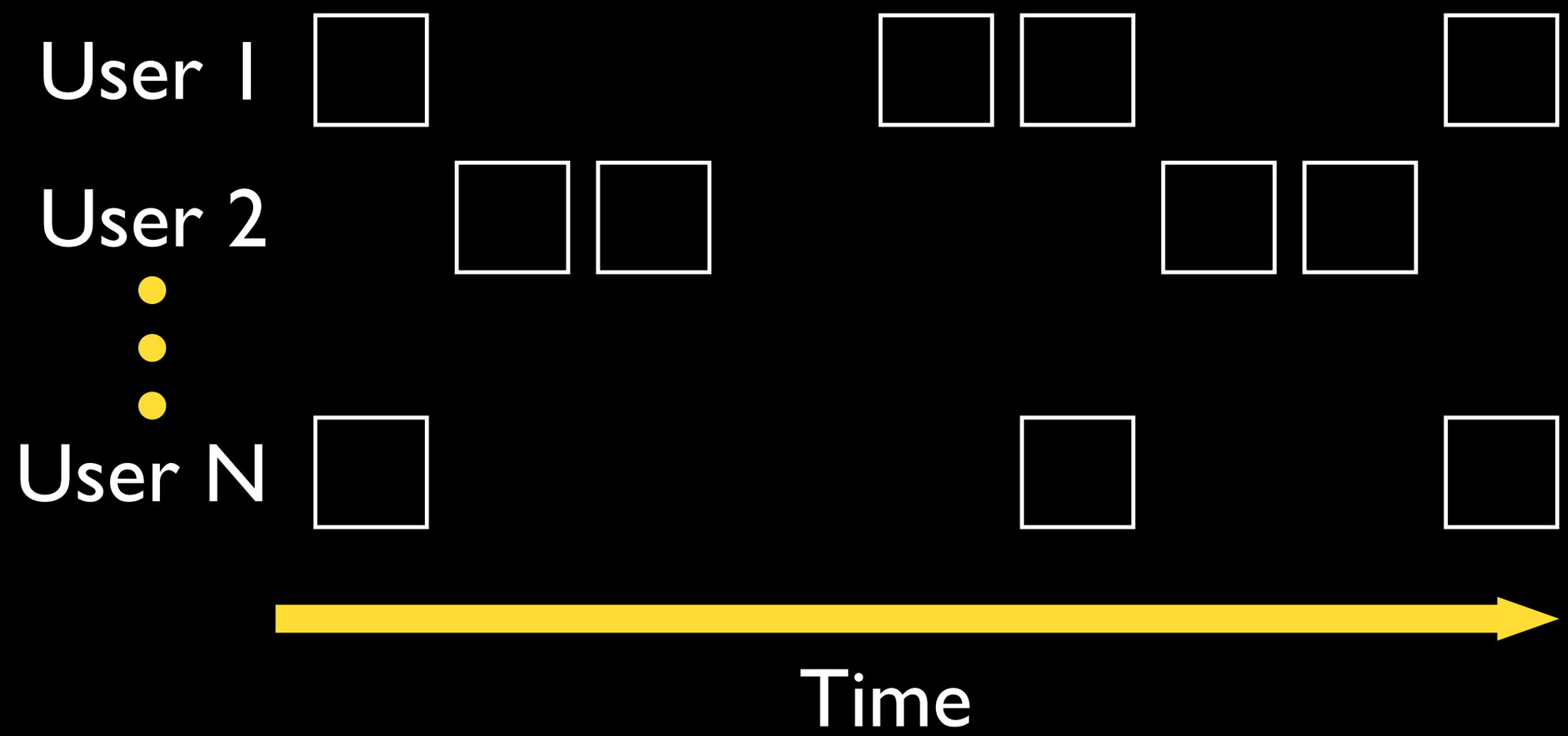
- Simulation Tool Use: Classroom Identification
- "and more" Resource Use
- Simulation Tool Use: Parameter Space Exploration

1: Classroom Identification

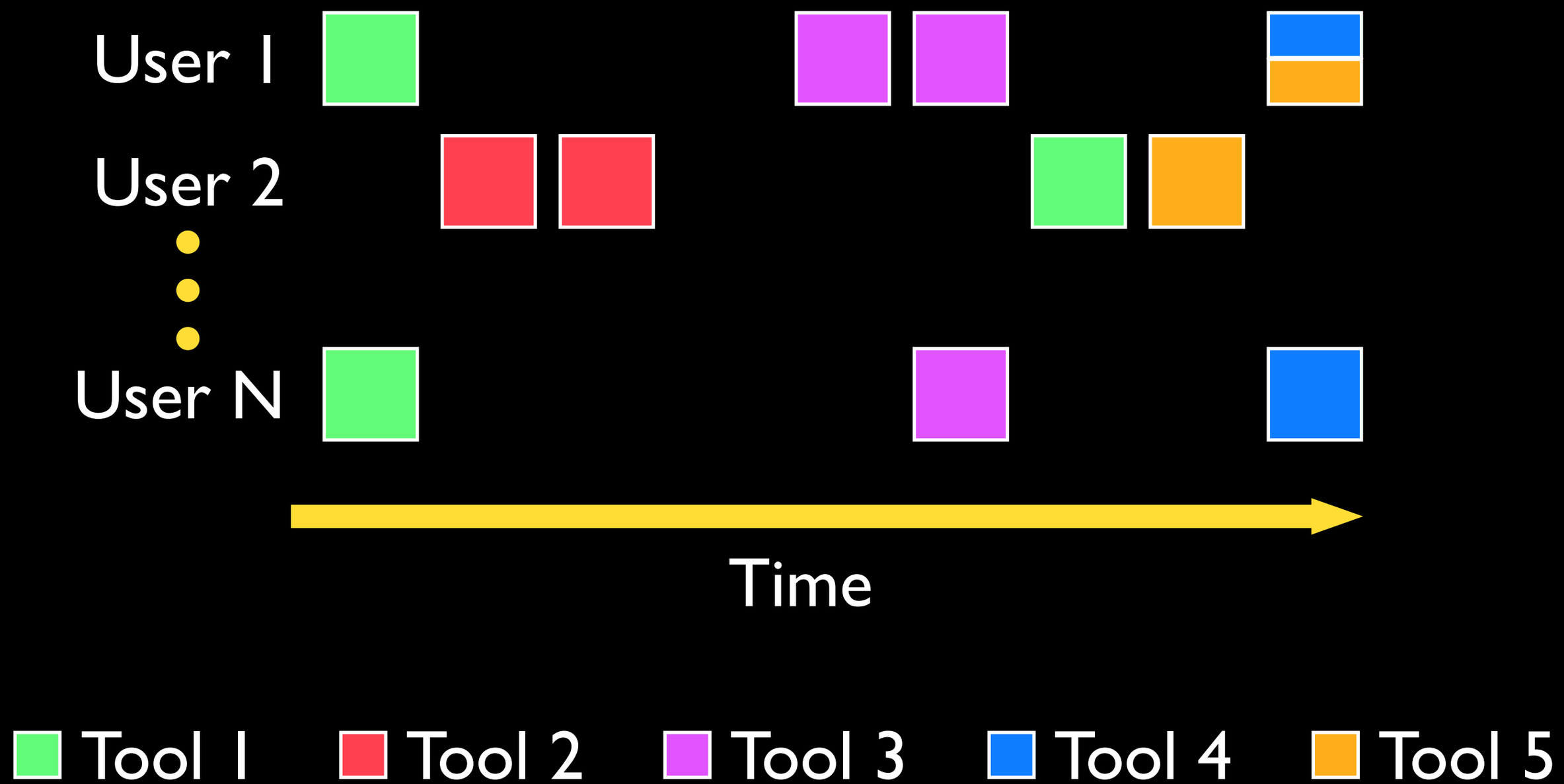
Hypothesis

Simulation tools are being used in more classroom settings than those of which we are aware.

1: Initial Exploration



1: Exploration

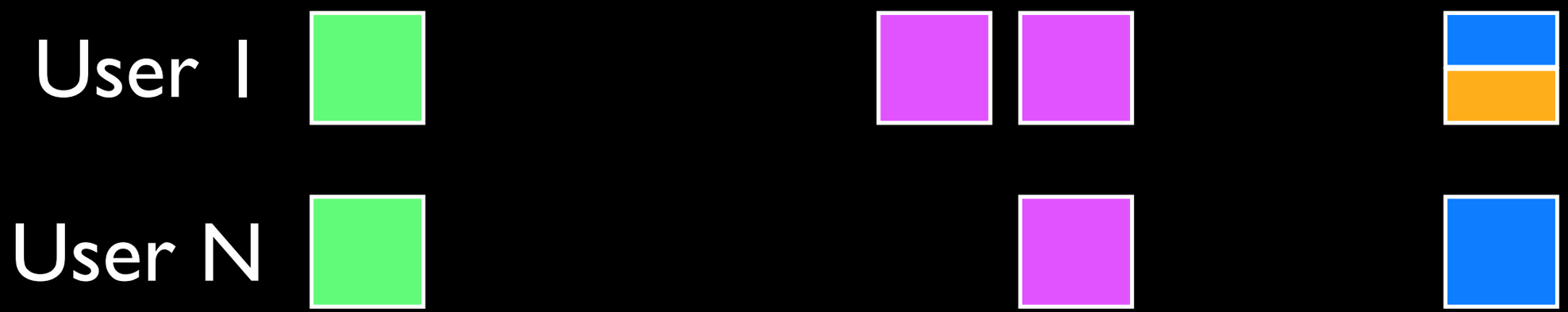


1: Identification

Pattern 1

Pattern 2

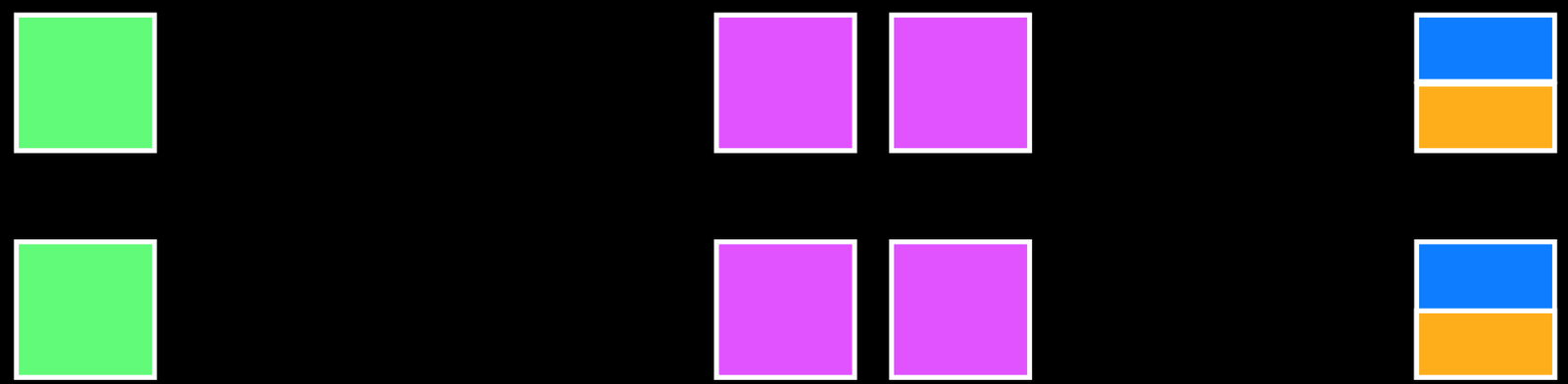
1: Characterization



1: Characterization

User 1

User N

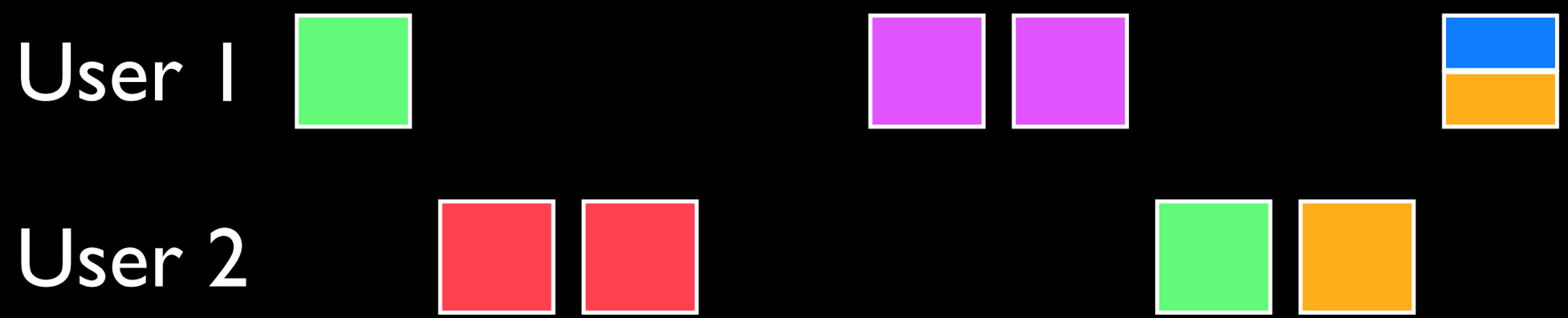


1: add orange
2: add purple

Penalties Assessed

|| = 3.04

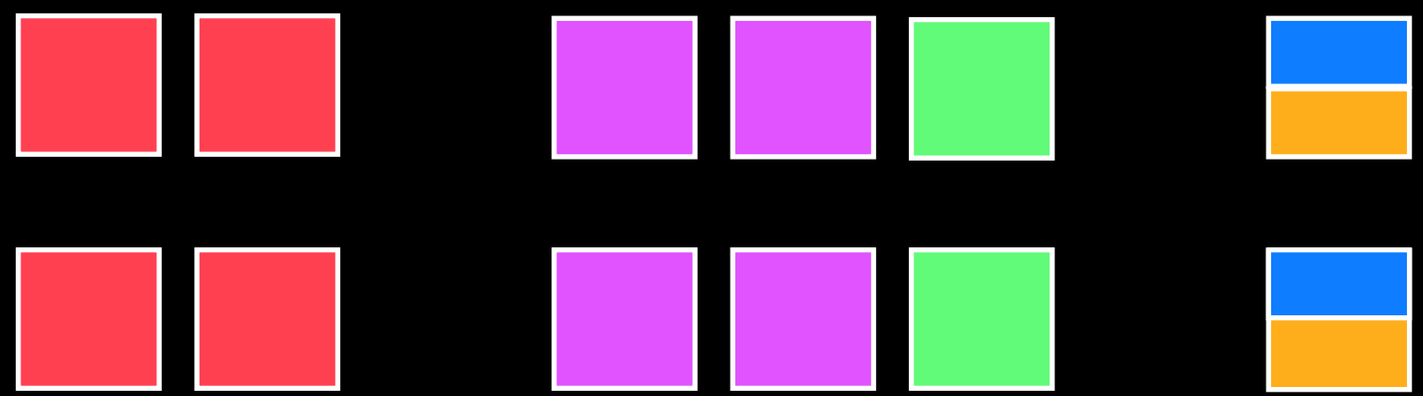
1: Characterization



1: Characterization

User 1

User 2

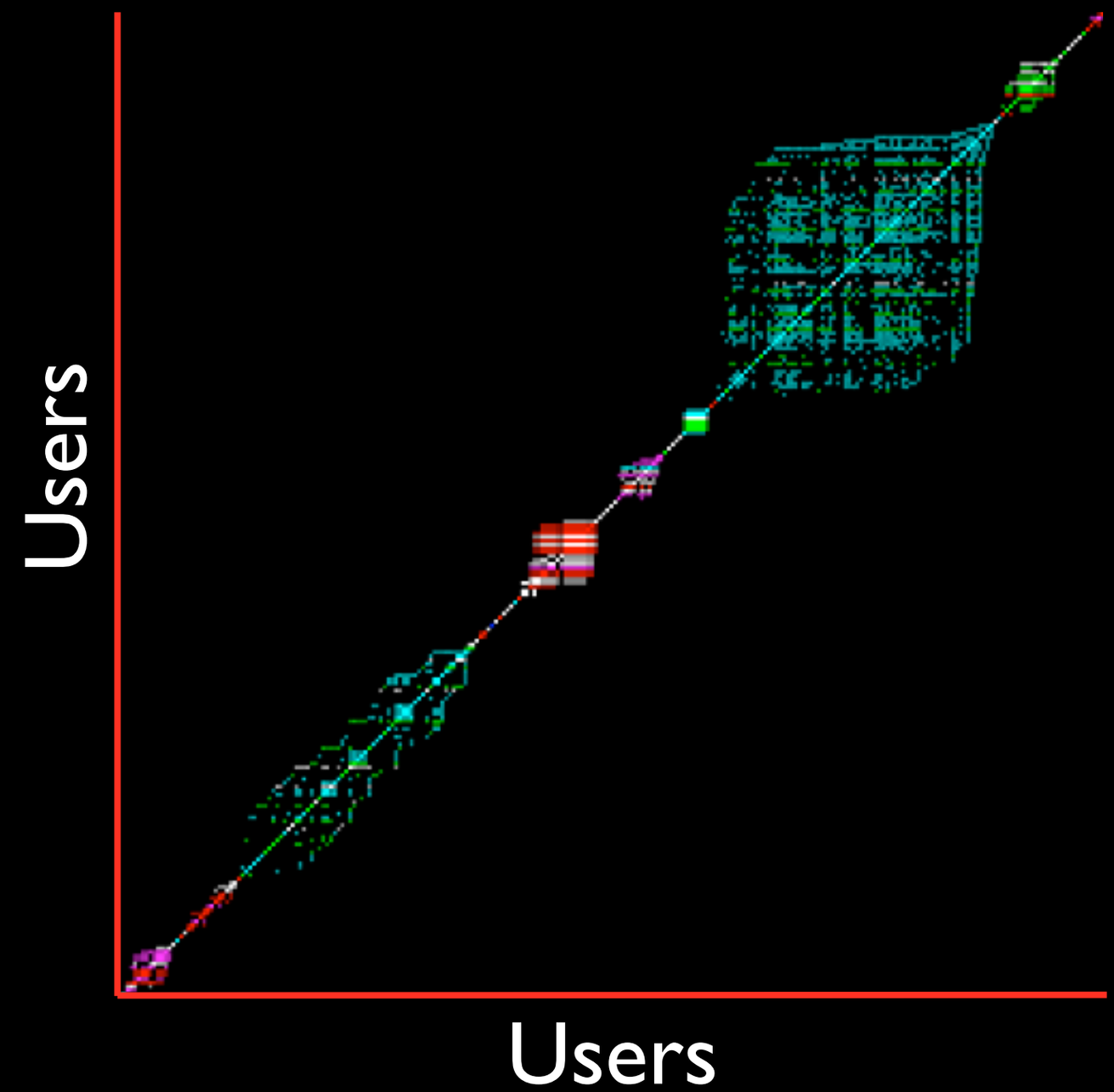


1: move orange
2: move green
3: add red
4: add red
5: add purple
6: add purple
7: add blue

Penalties Assessed

~~IIII~~ II = 25.6

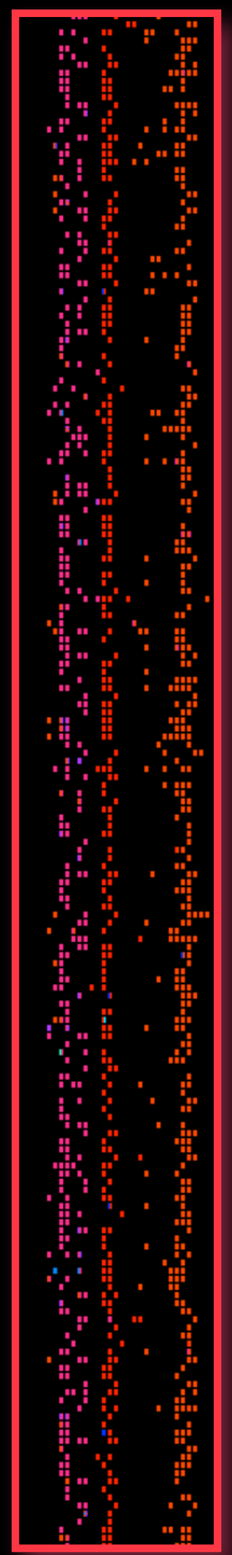
1: Characterization



Dot intensity is the strength of User-User similarity

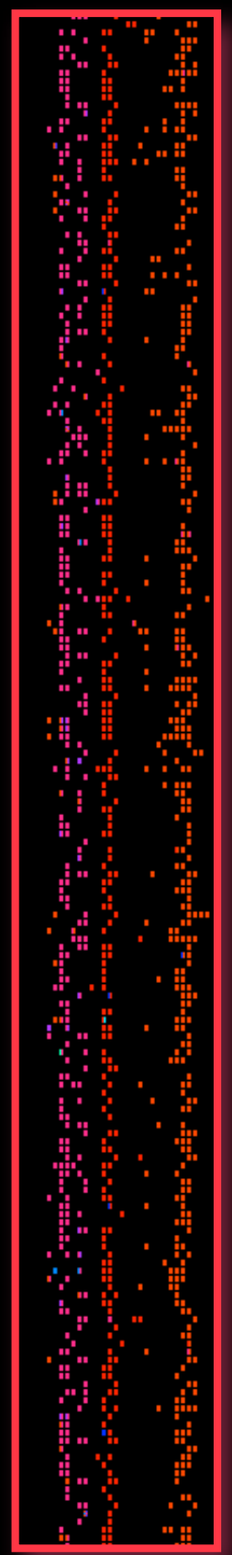
Existence of clusters becomes evident

1:Visualization



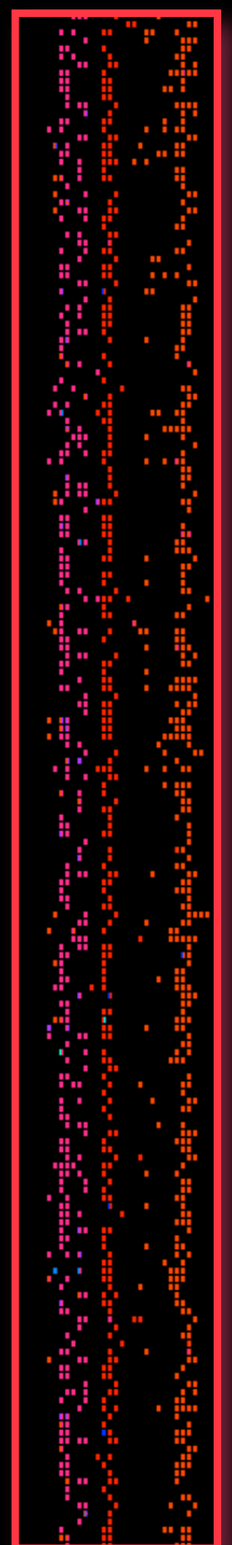
Large Group
Multiple Tools
Moderate Re-use

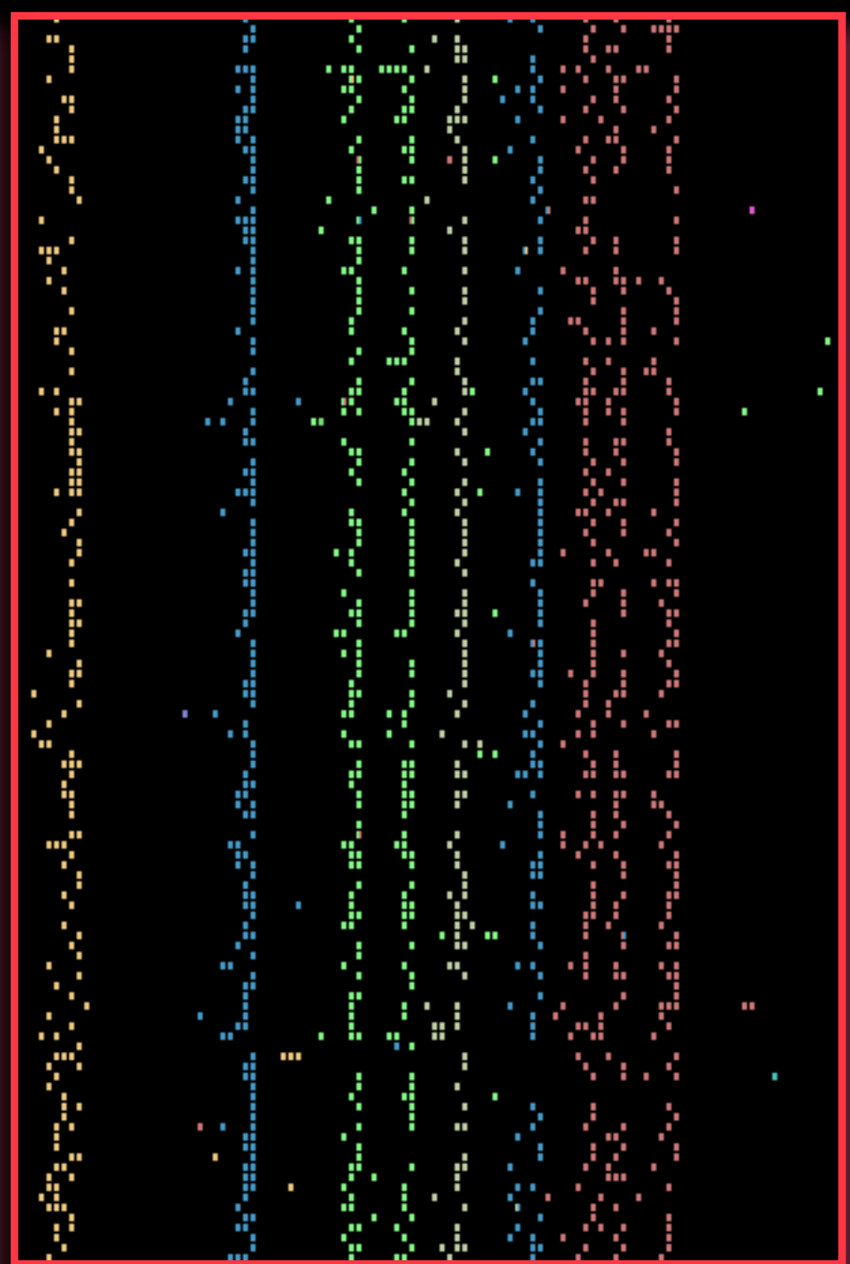
1:Visualization



Large Group
Single Tool
Heavy Re-use

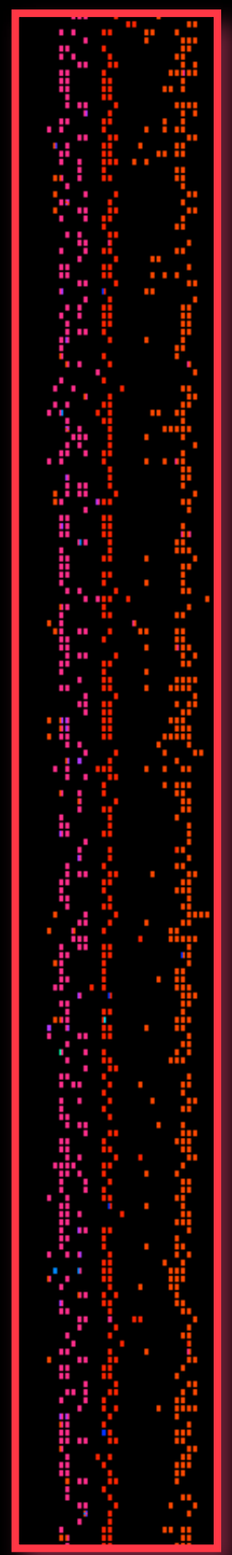
1:Visualization

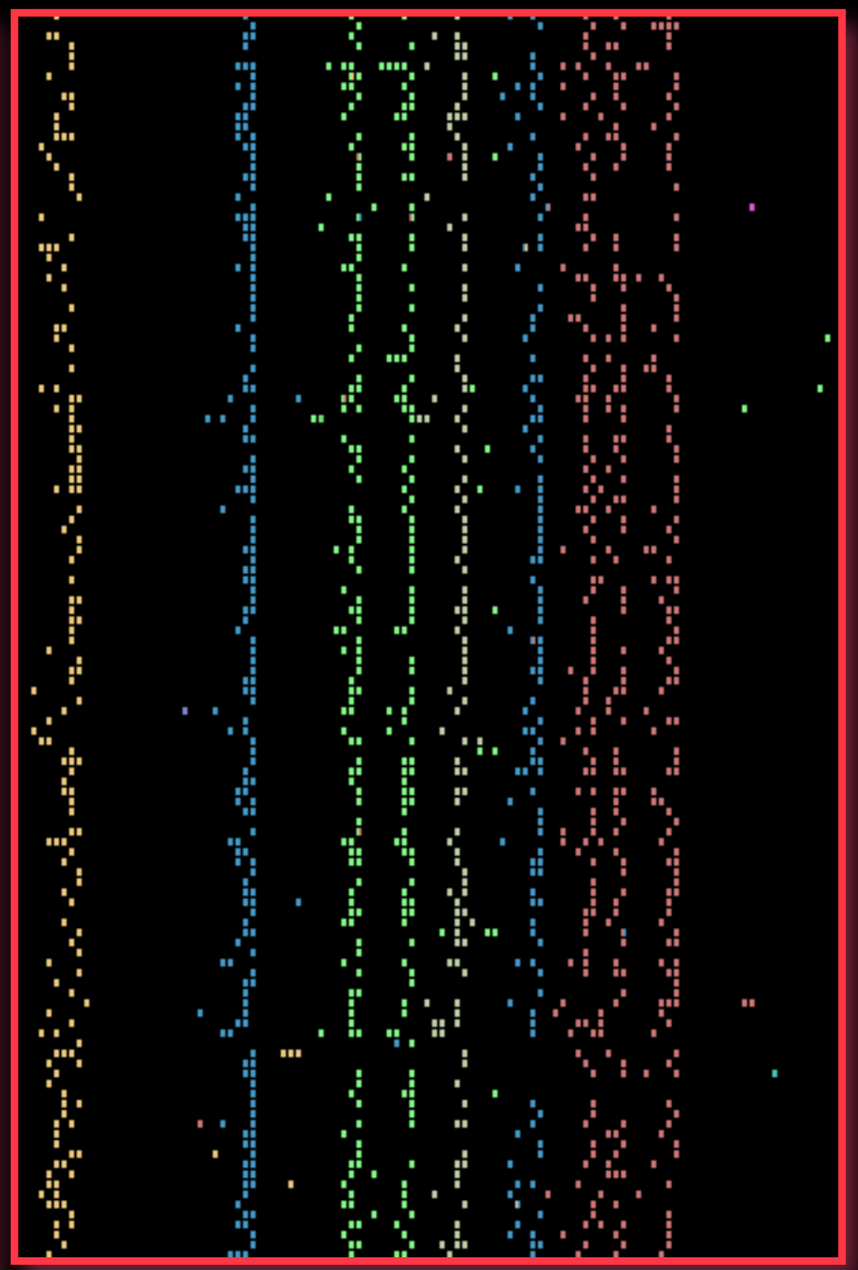




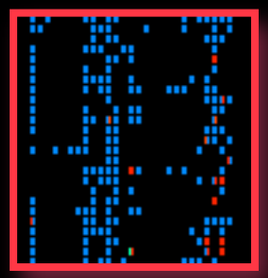
Large Group
Multiple Tool
Periodic
Re-use

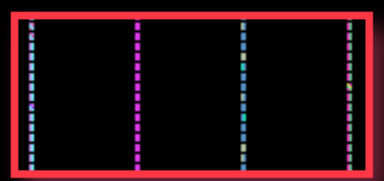
1:Visualization





Small Groups
Intense or
Periodic Use





1: Publication

- Immediate impact on nanoHUB.org
- Peer review & scientific recognition

Usage: Tools

Overview | Tools | Maps

Show data for: Top Tools by Users in Courses

Top Tools by Users in Courses

#	Tool		
1	QC-Lab		
2	Nanosphere Optics Lab		
3	PN Junction Lab		
4	MOSCap		
5	Quantum Dot Lab		
6	Crystal Viewer Tool		
7	Illinois Solid State Electronic Device		
8	CNDO/INDO		
9	Spice3f4		
10	MOSFet		
11	ABACUS - Assembly of Basic Applications for Coordinated Understanding of Semiconductors	524	4.47%
12	Band Structure Lab	694	3.77%
13	Drift-Diffusion Lab	660	3.58%
14	FETToy	644	3.50%
15	BJT Lab	622	3.38%

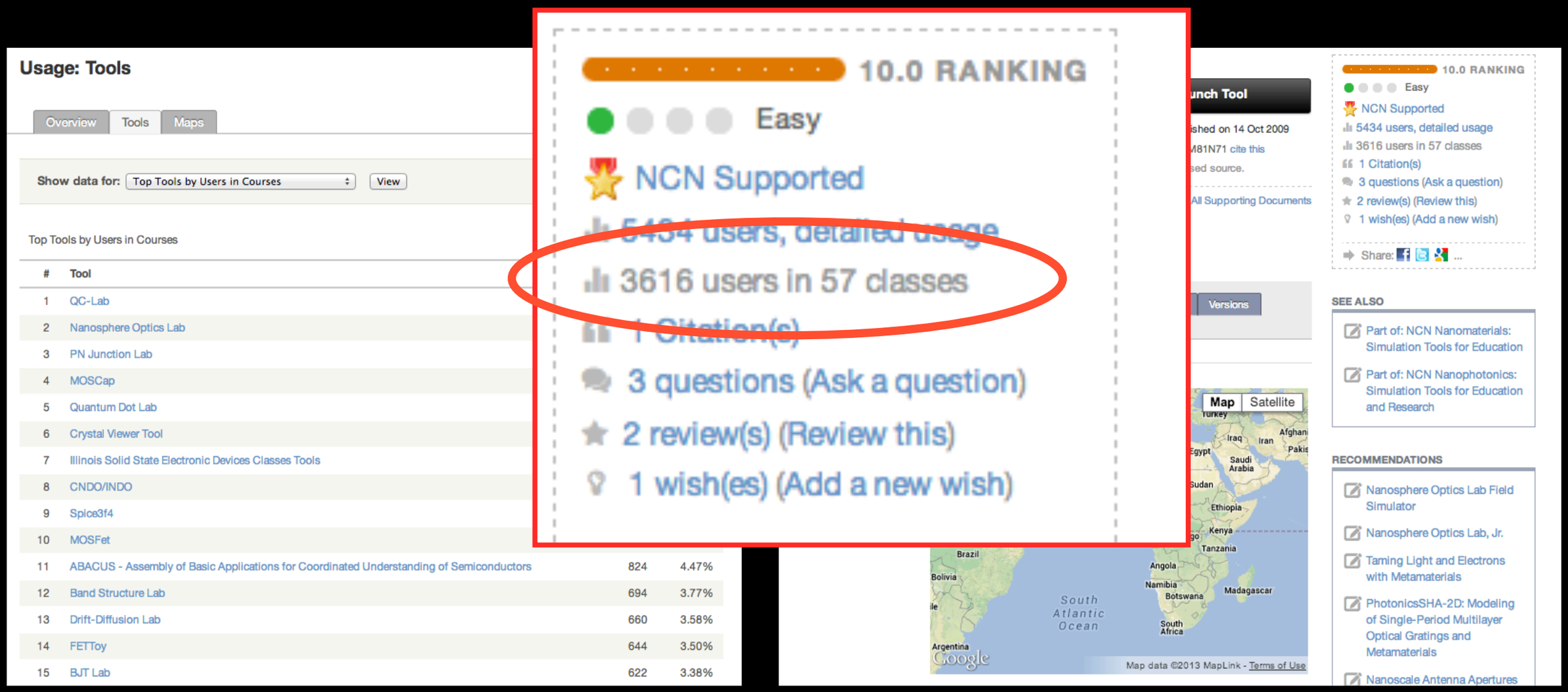
Show data for: Top Tools by Users in Courses | View

Top Tools by Users in Courses

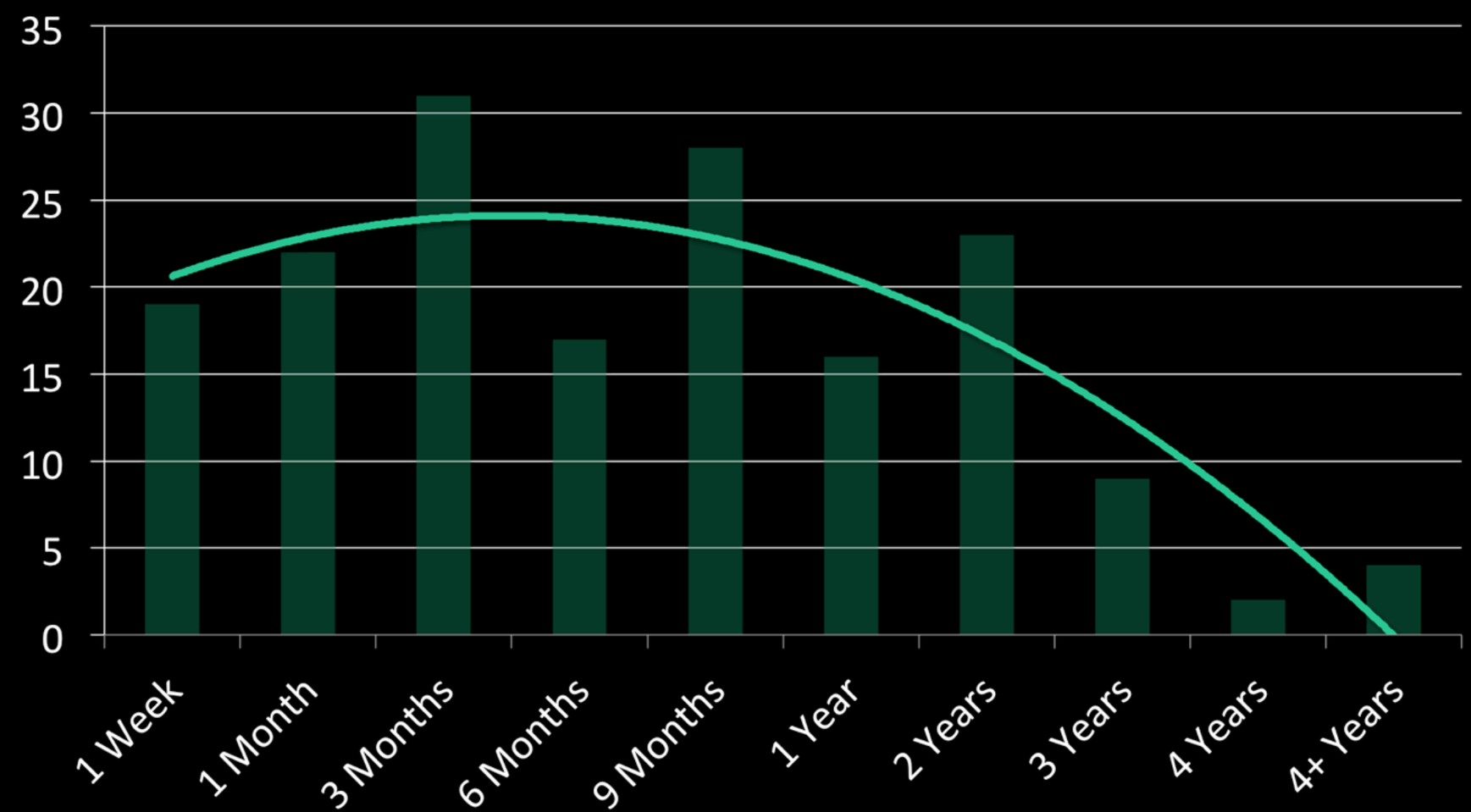
#	Tool	Users in Courses	Percent
1	QC-Lab	3,981	21.61%
2	Nanosphere Optics Lab	3,616	19.63%
3	PN Junction Lab	2,597	14.10%
4	MOSCap	1,312	7.12%
5	Quantum Dot Lab	1,117	6.06%
6	Crystal Viewer Tool	1,071	5.81%

1: Publication

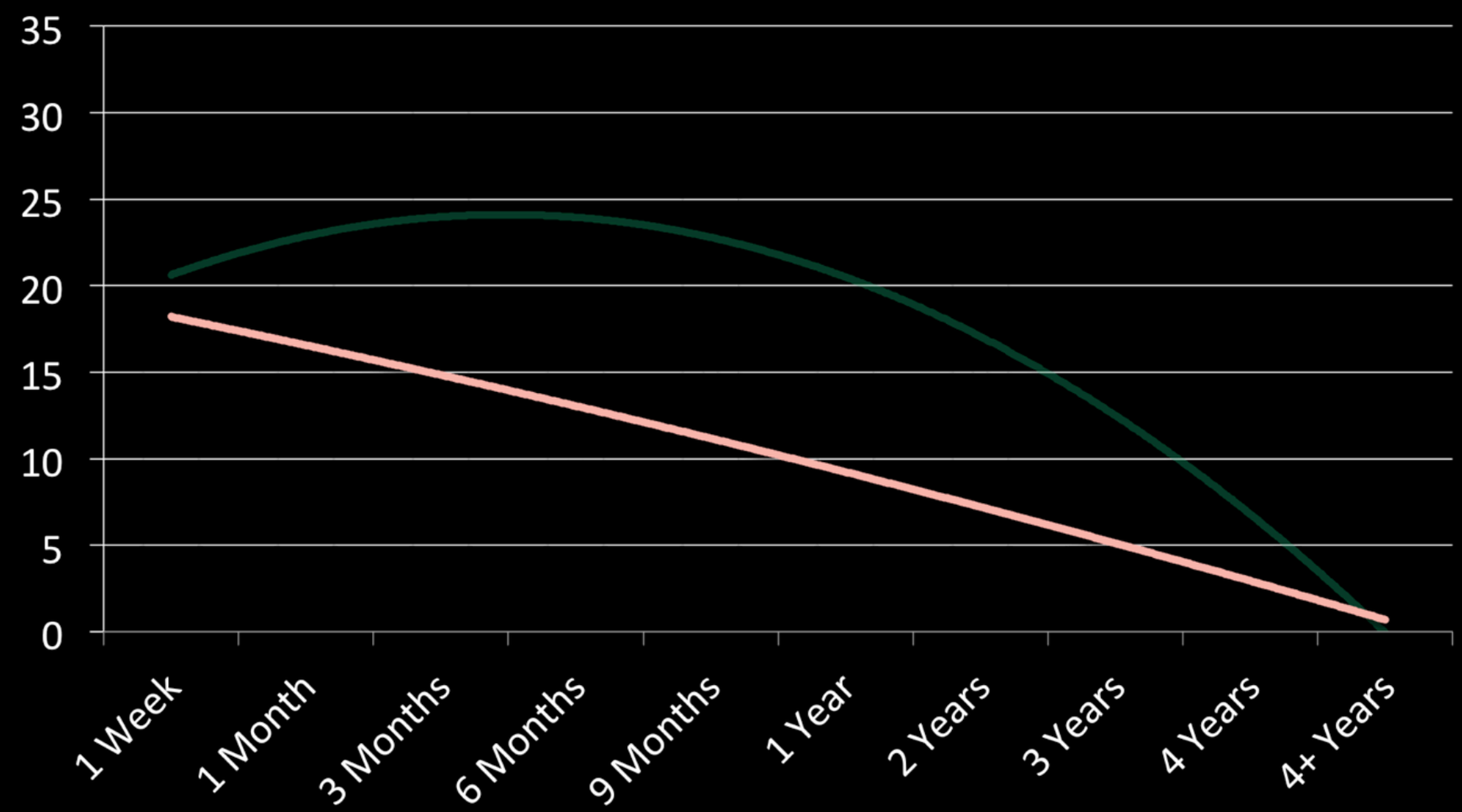
- Immediate impact on nanoHUB.org
- Peer review & scientific recognition



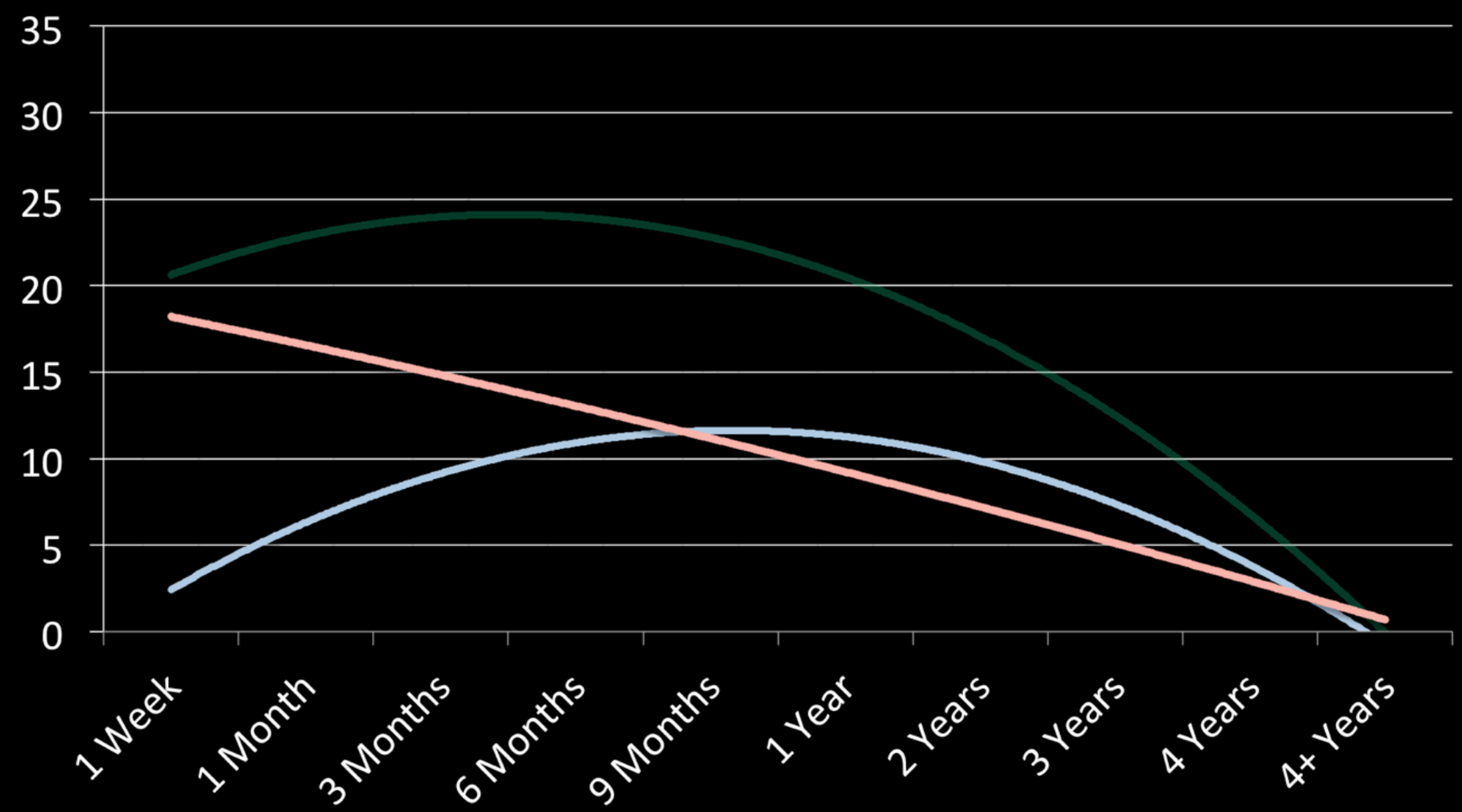
1: Impact - Adoption



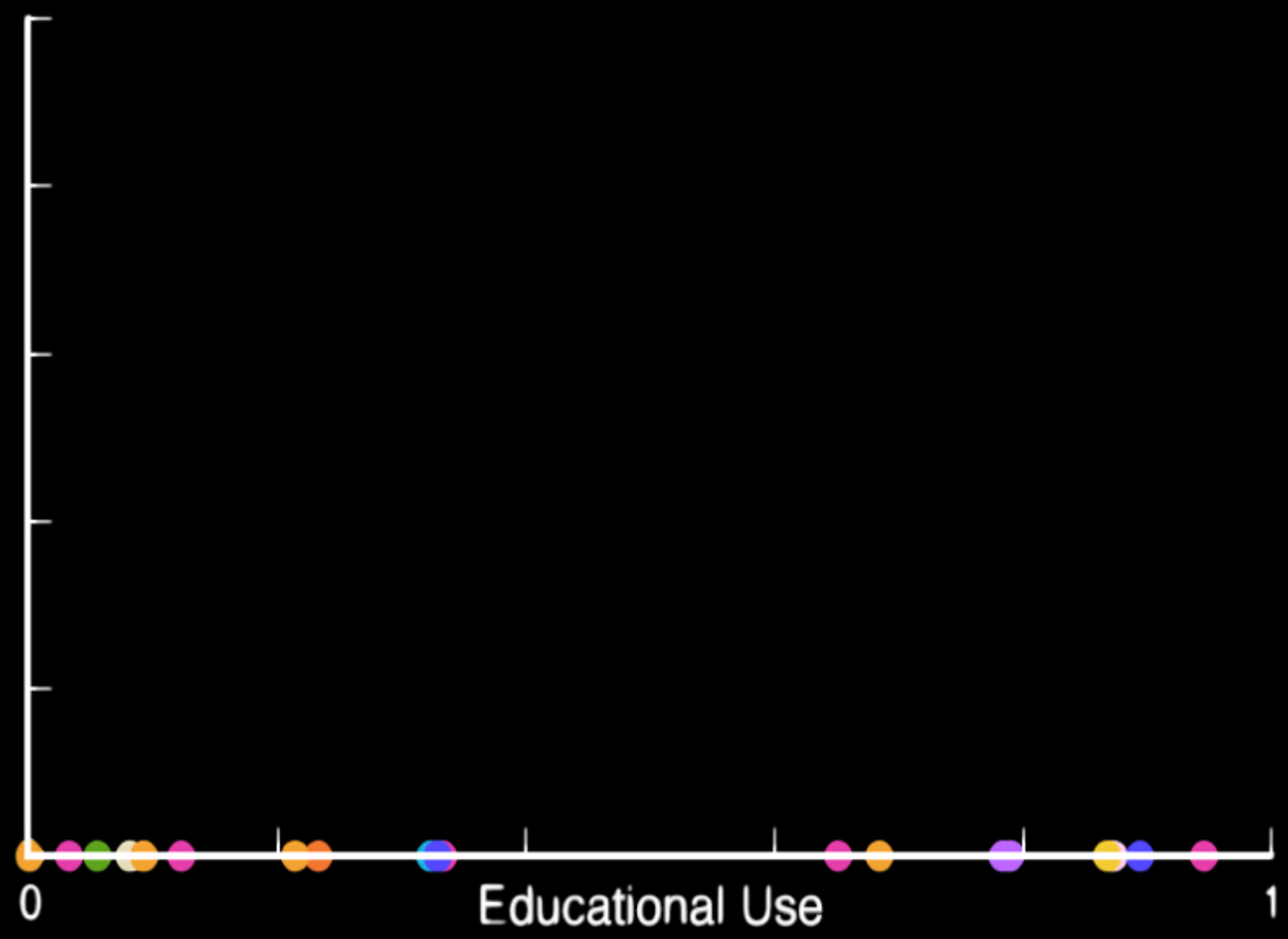
1: Impact - Adoption



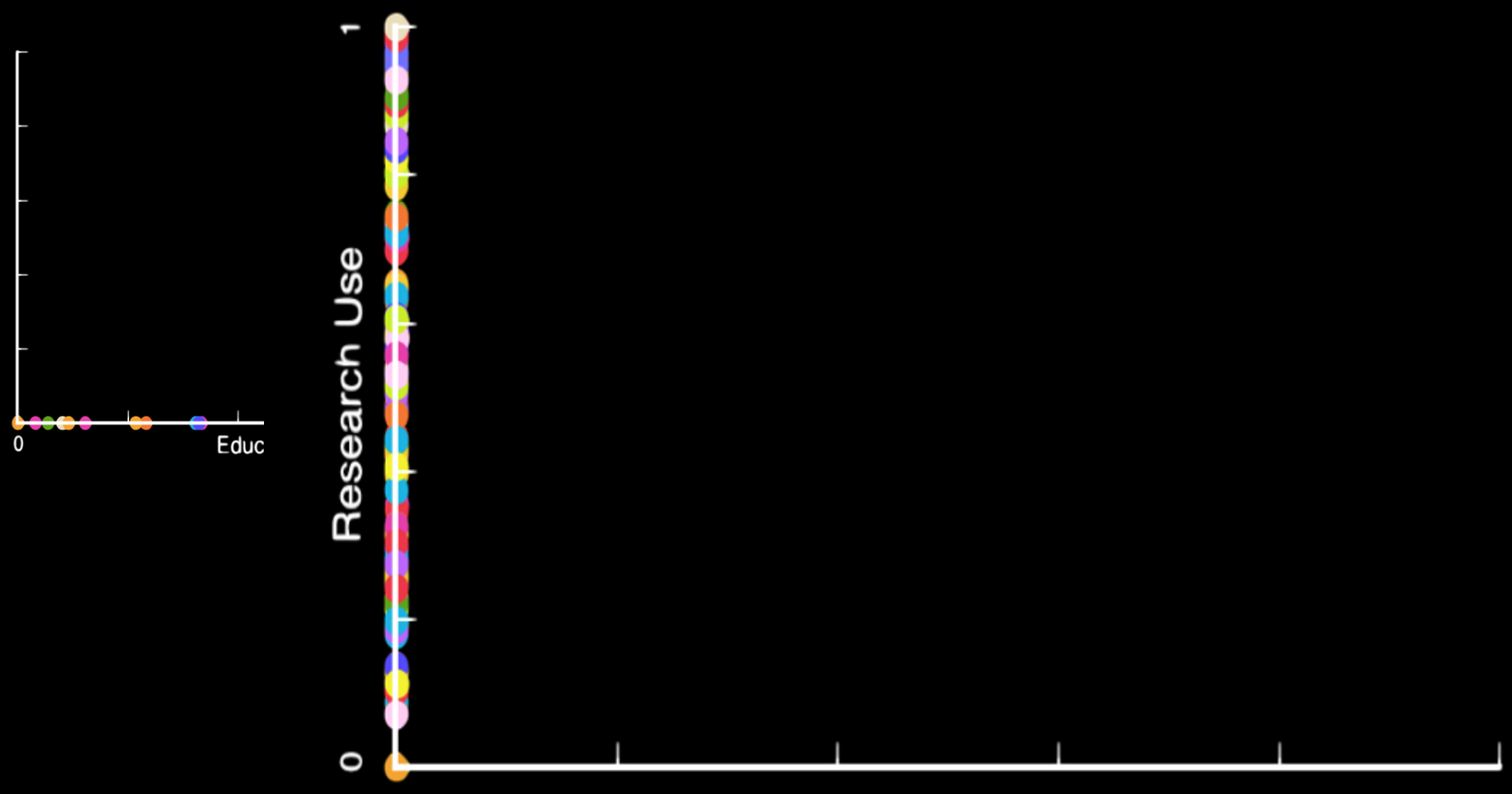
1: Impact - Adoption



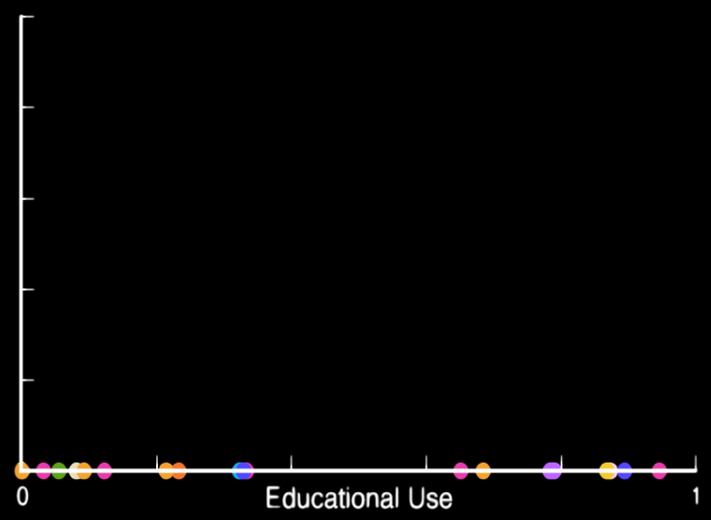
1: Impact - Migration

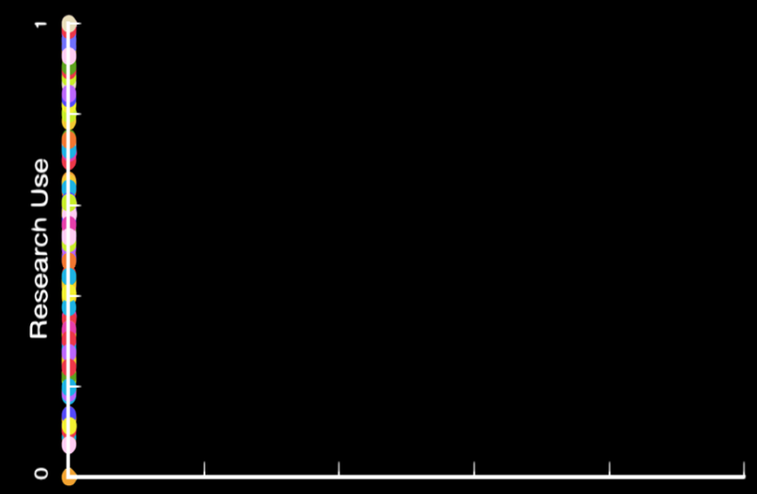


1: Impact - Migration

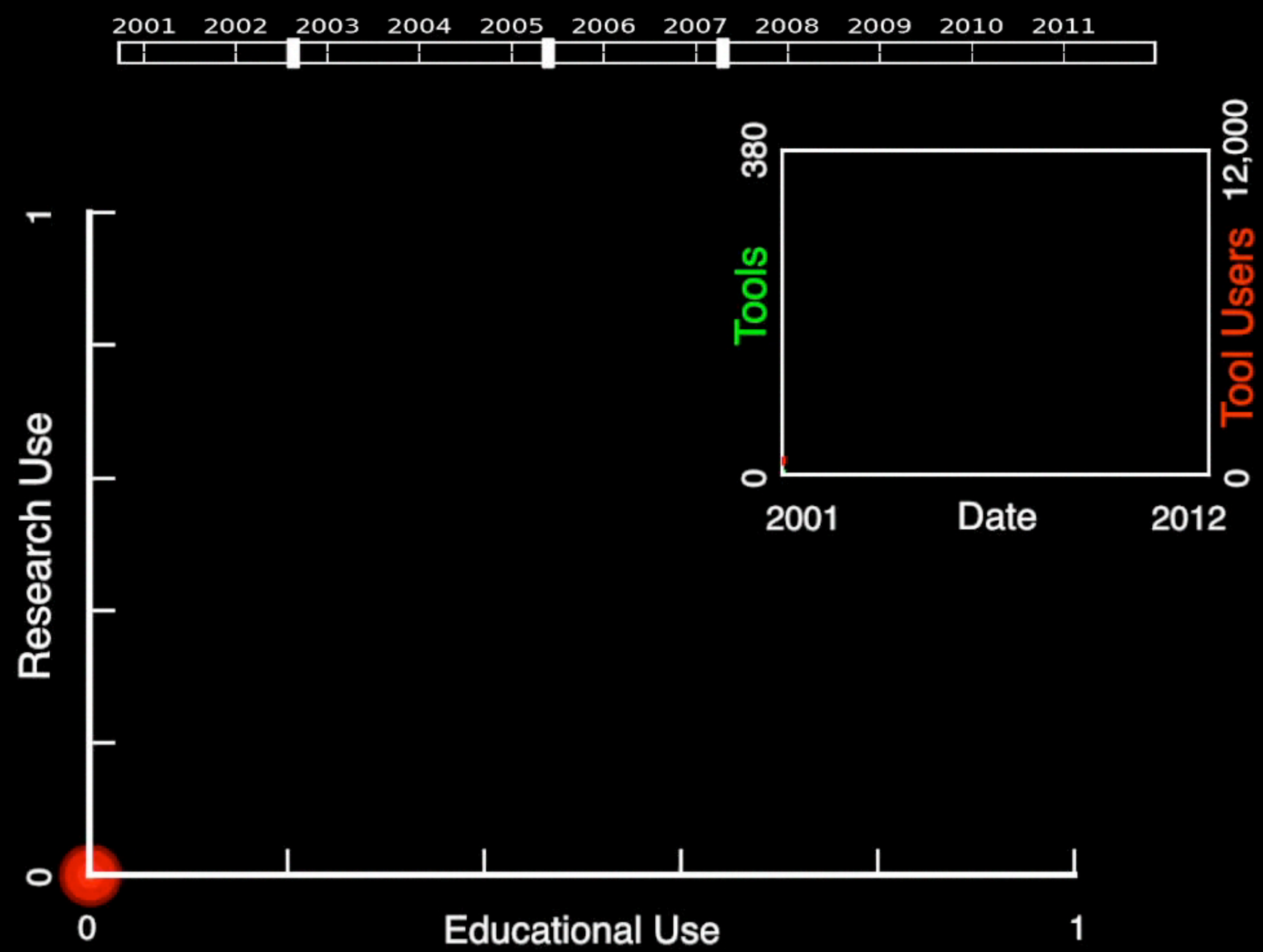


1: Impact - Migration



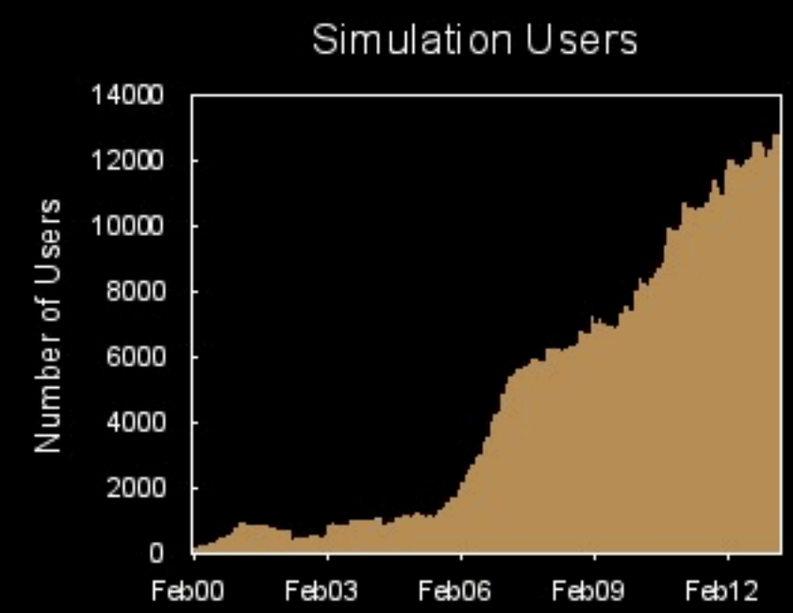


1: Impact - Migration

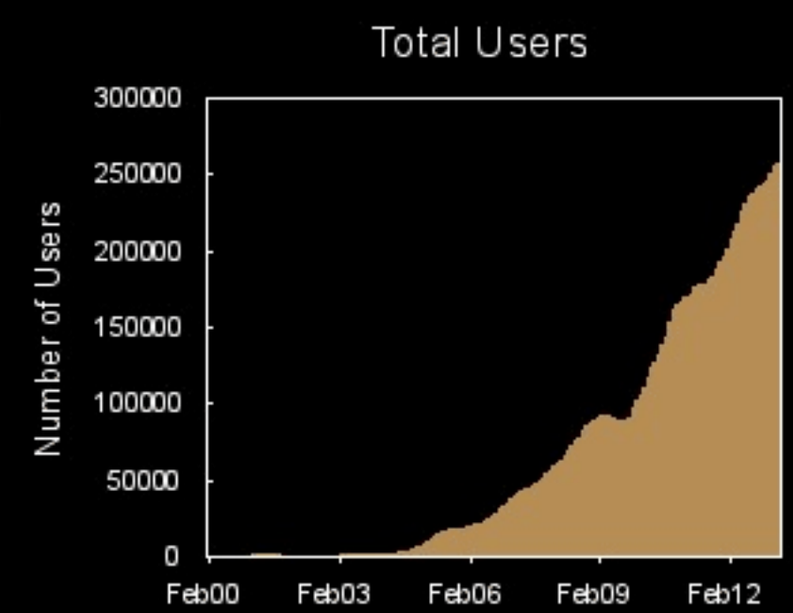


2: "and more" Usage

- Simulation Tools (> 12,000 users/yr)
  - Requires Login
  - All Human Generated Activity
  - Easy to Track Longitudinal Activity



- "and more" Content (>257,000 users/yr)
  - Free Access
  - Human AND Robotic Generated Activity
  - Difficult to Track Longitudinal Activity



What might "and more" users tell us differently than tool users?

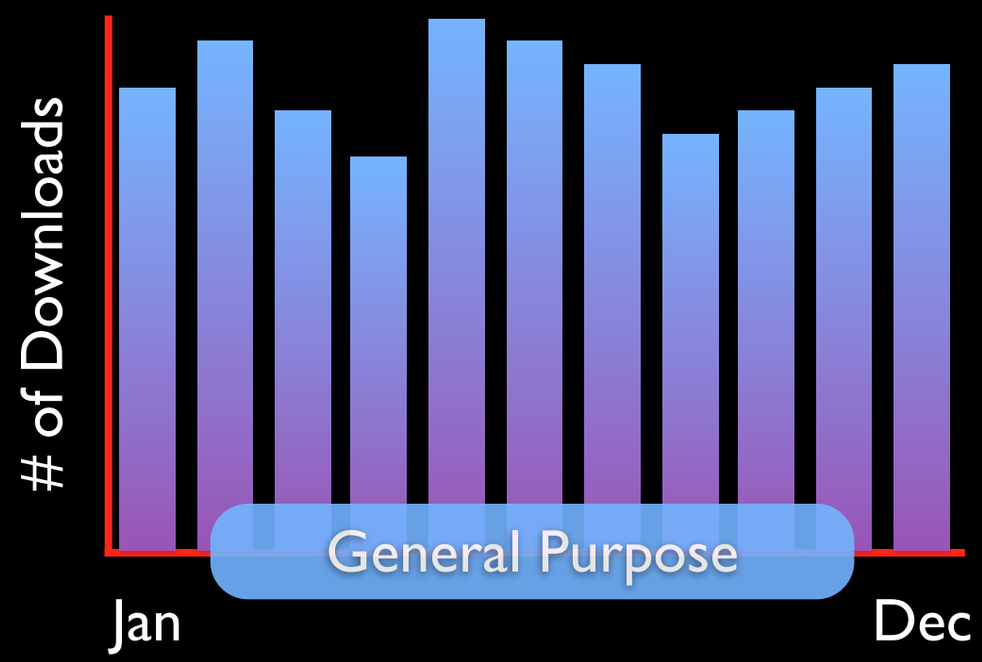
2: non-Human Activity

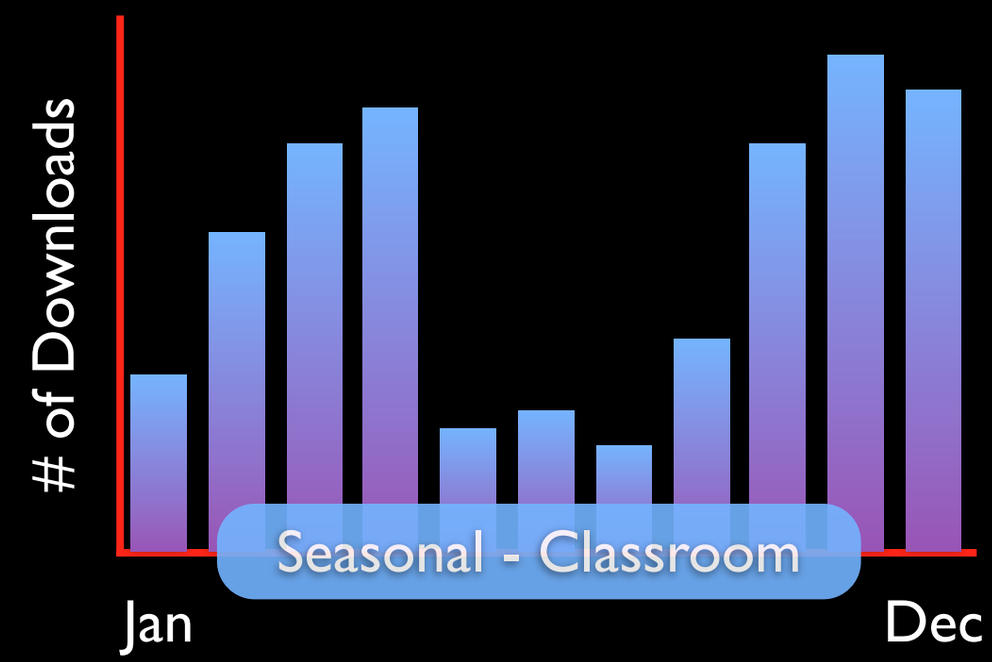
Example: 2011 data

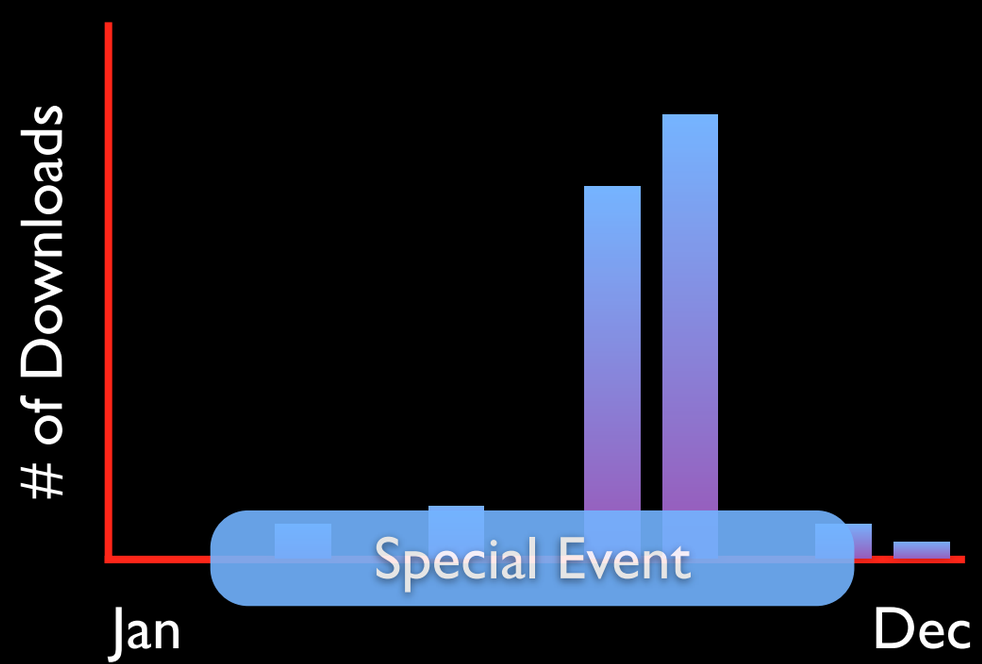
"and more" downloads/plays	1,641,007
Known robots (> 17,000)	-397,939
Automatic detection methods	-567,228
Human generated downloads	675,840

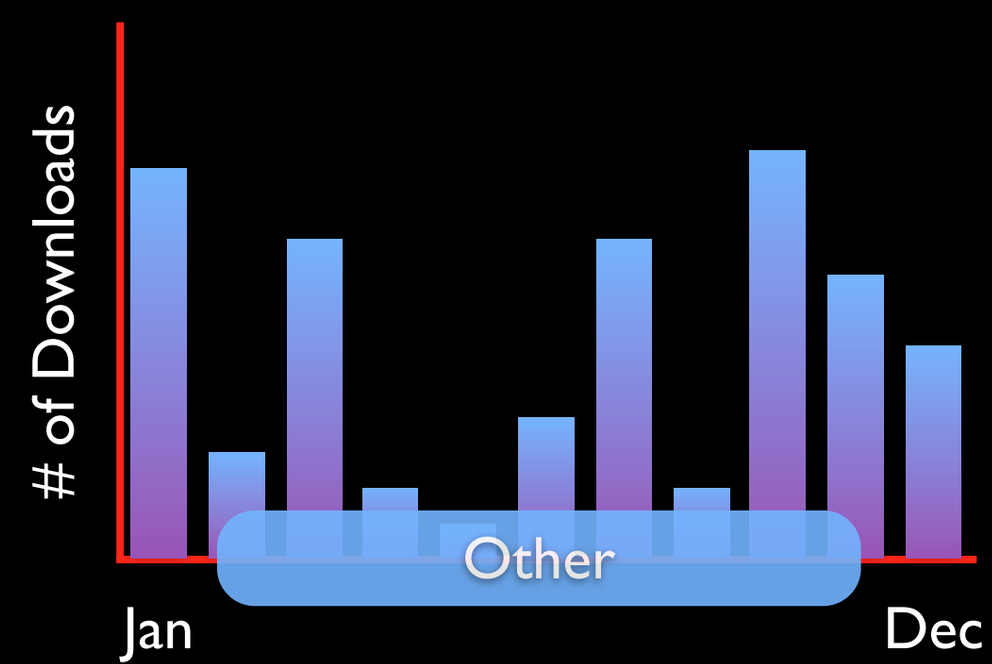
2: Exploration

Hypotheses of Patterns



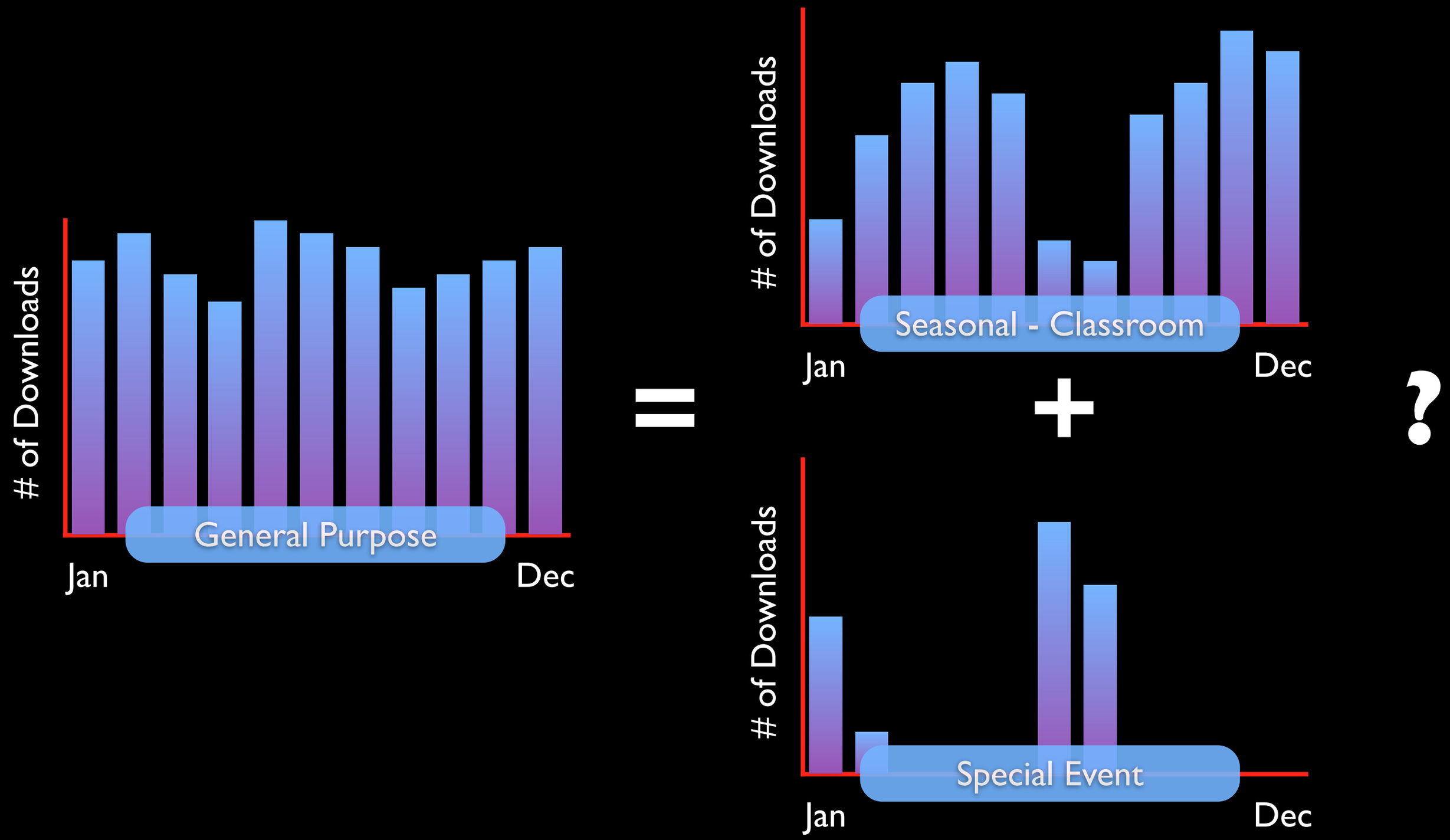






2: Exploration

Combinations of Patterns

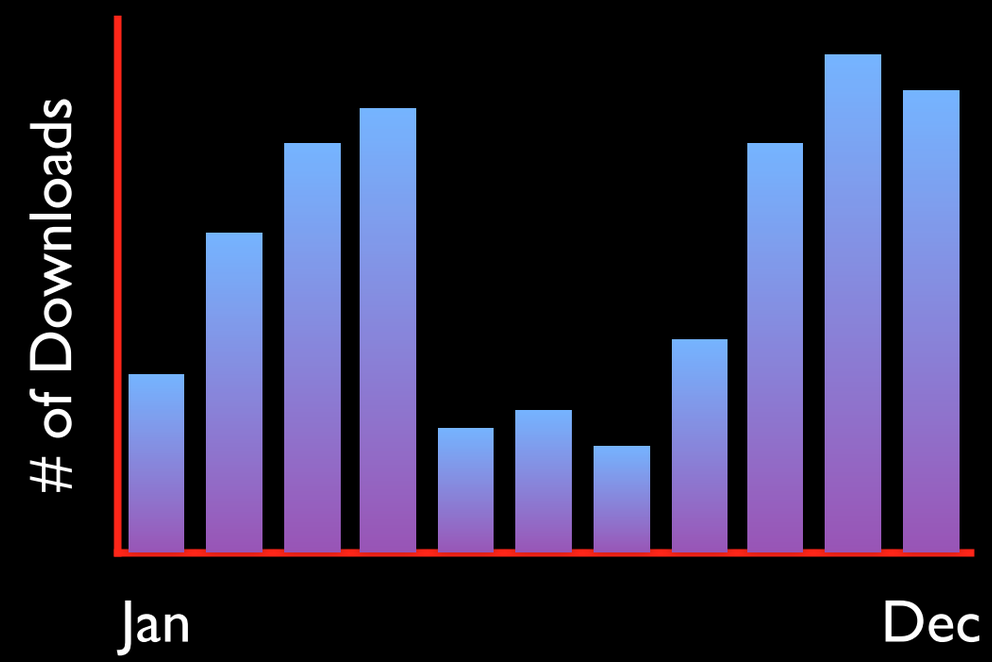


2:Visualization

How to visualize "pure" patterns
and additive combined patterns?

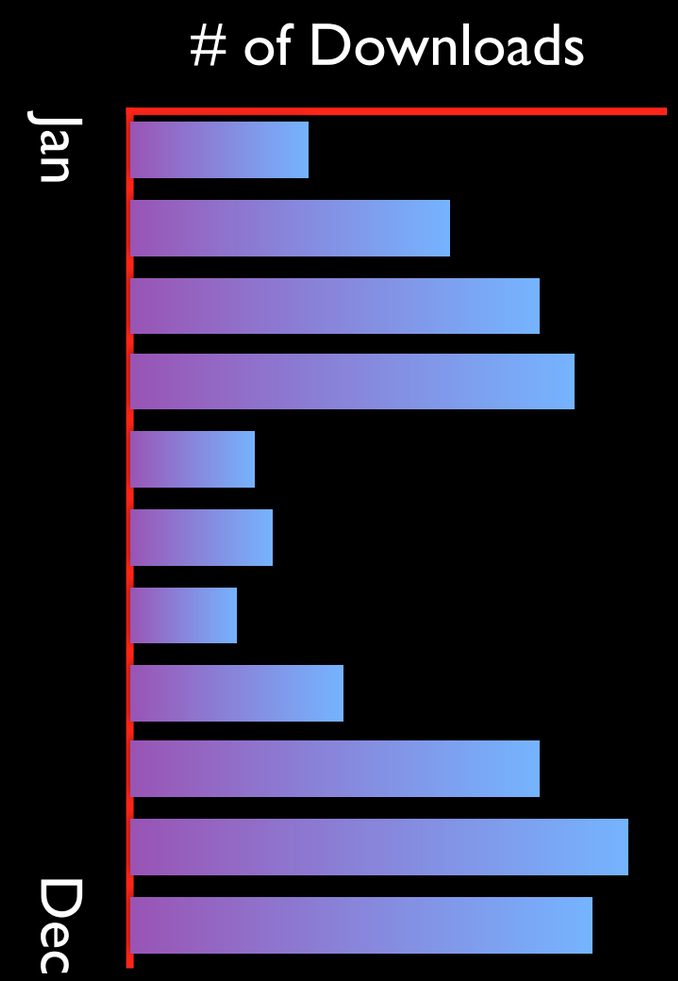
Spatial

+

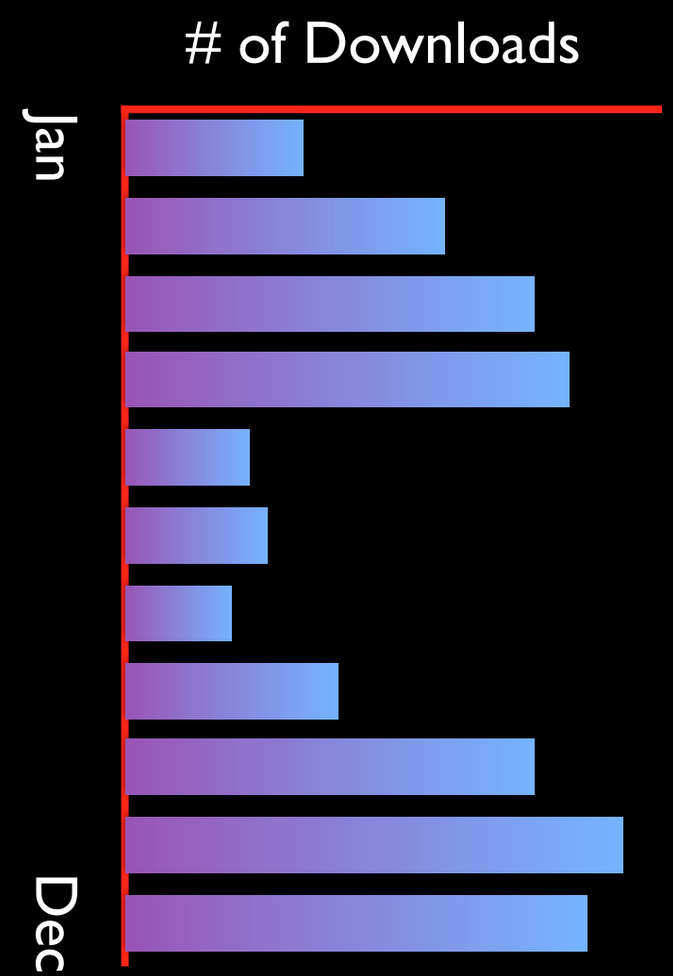


Temporal

2:Visualization

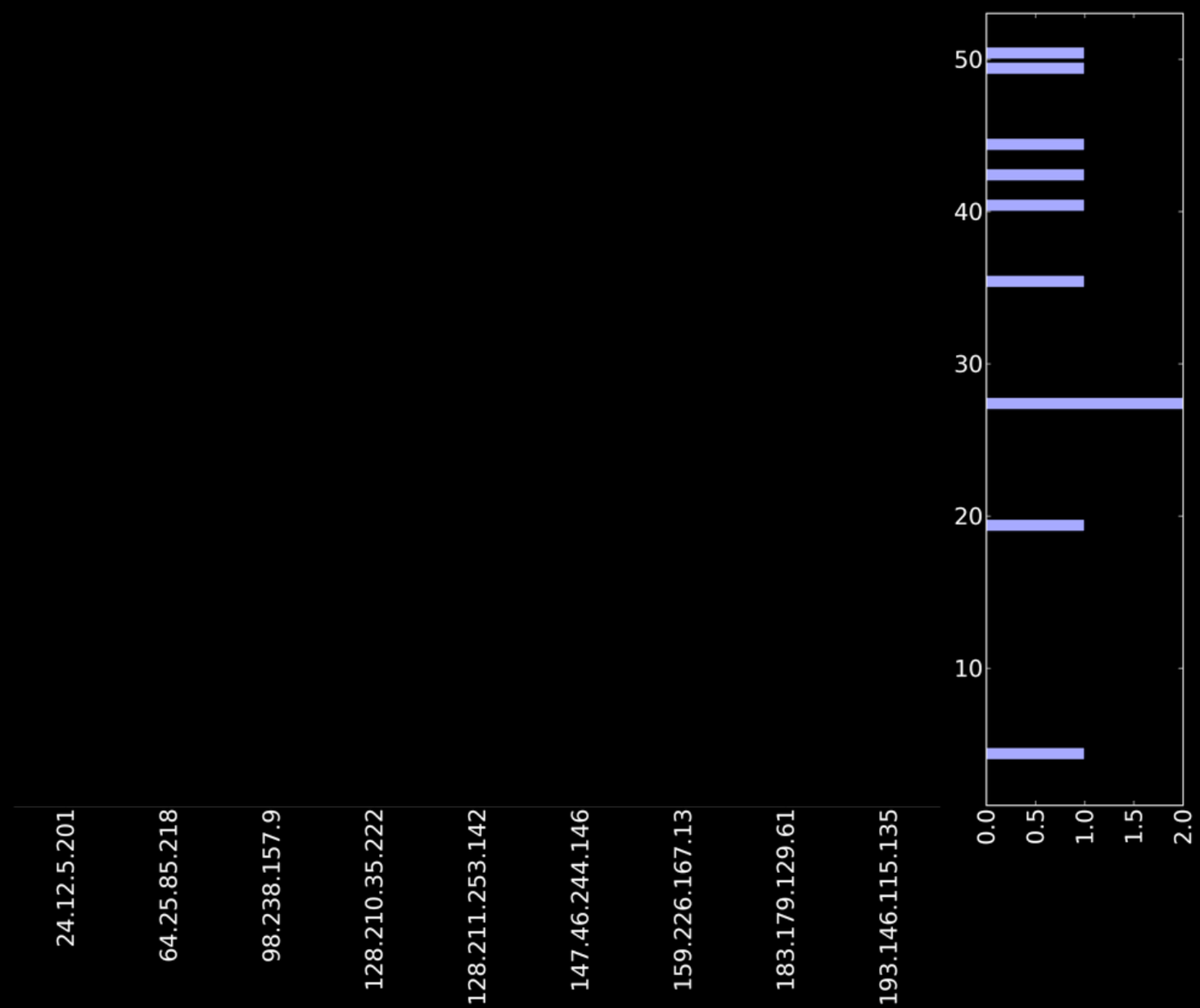


2:Visualization

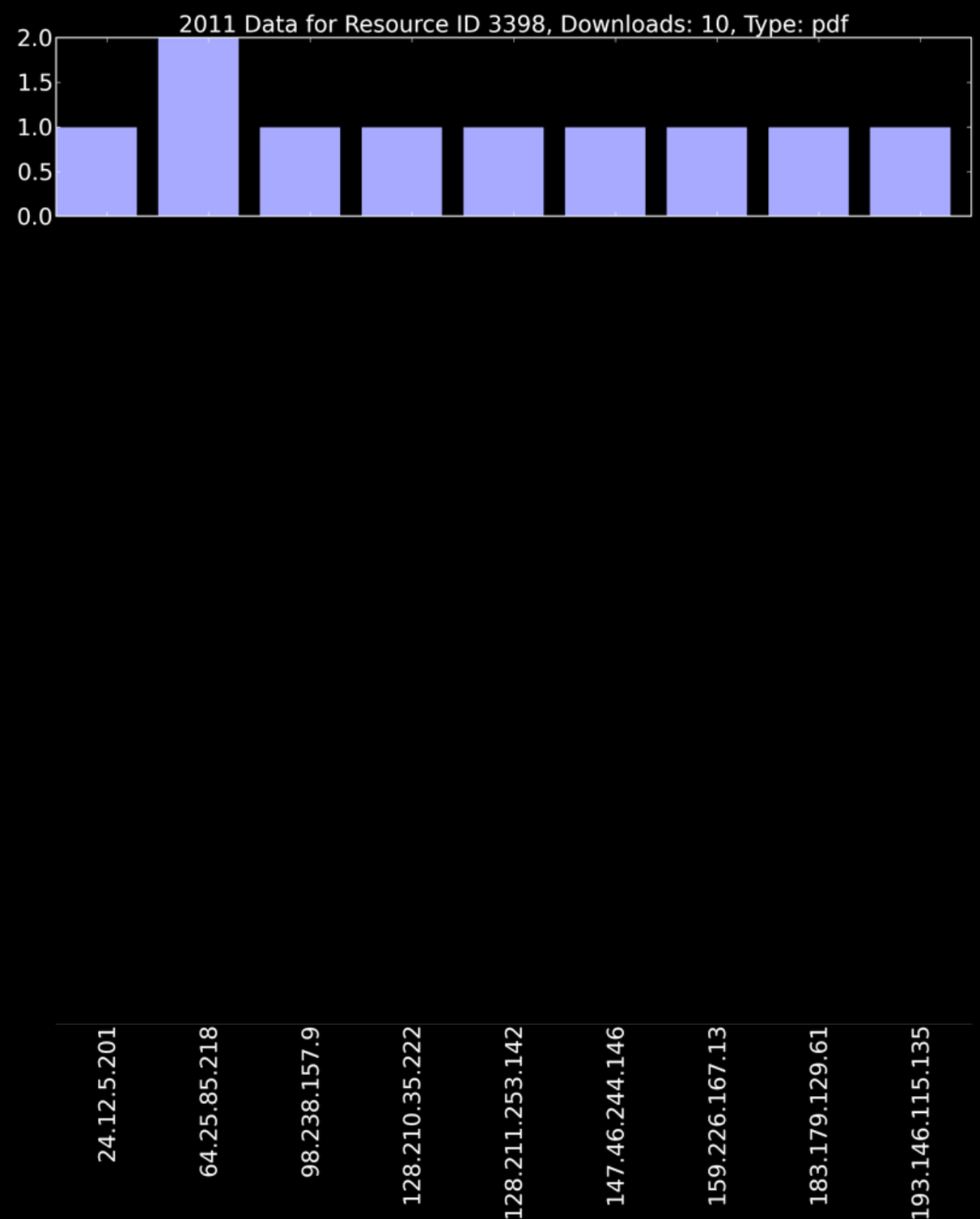


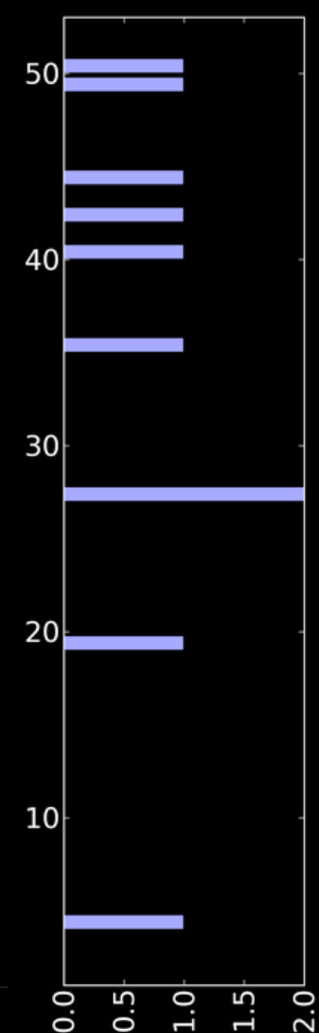
123.125.67.243
123.125.68.95
220.181.18.12
220.181.18.13
220.181.27.12
220.181.27.13
220.181.37.85
220.181.51.217
220.181.51.218
220.181.51.219
220.181.51.220

2:Visualization

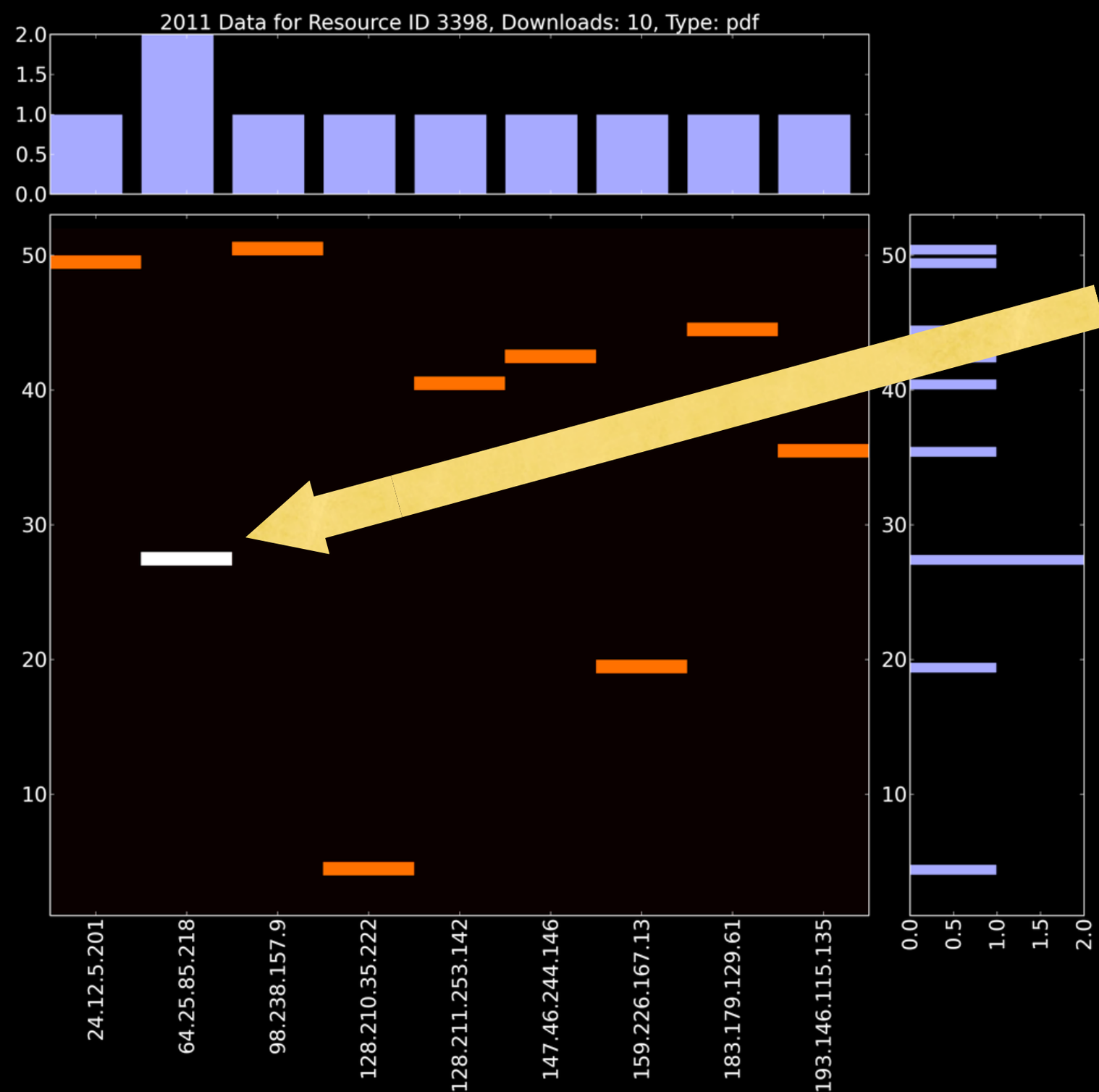


2:Visualization



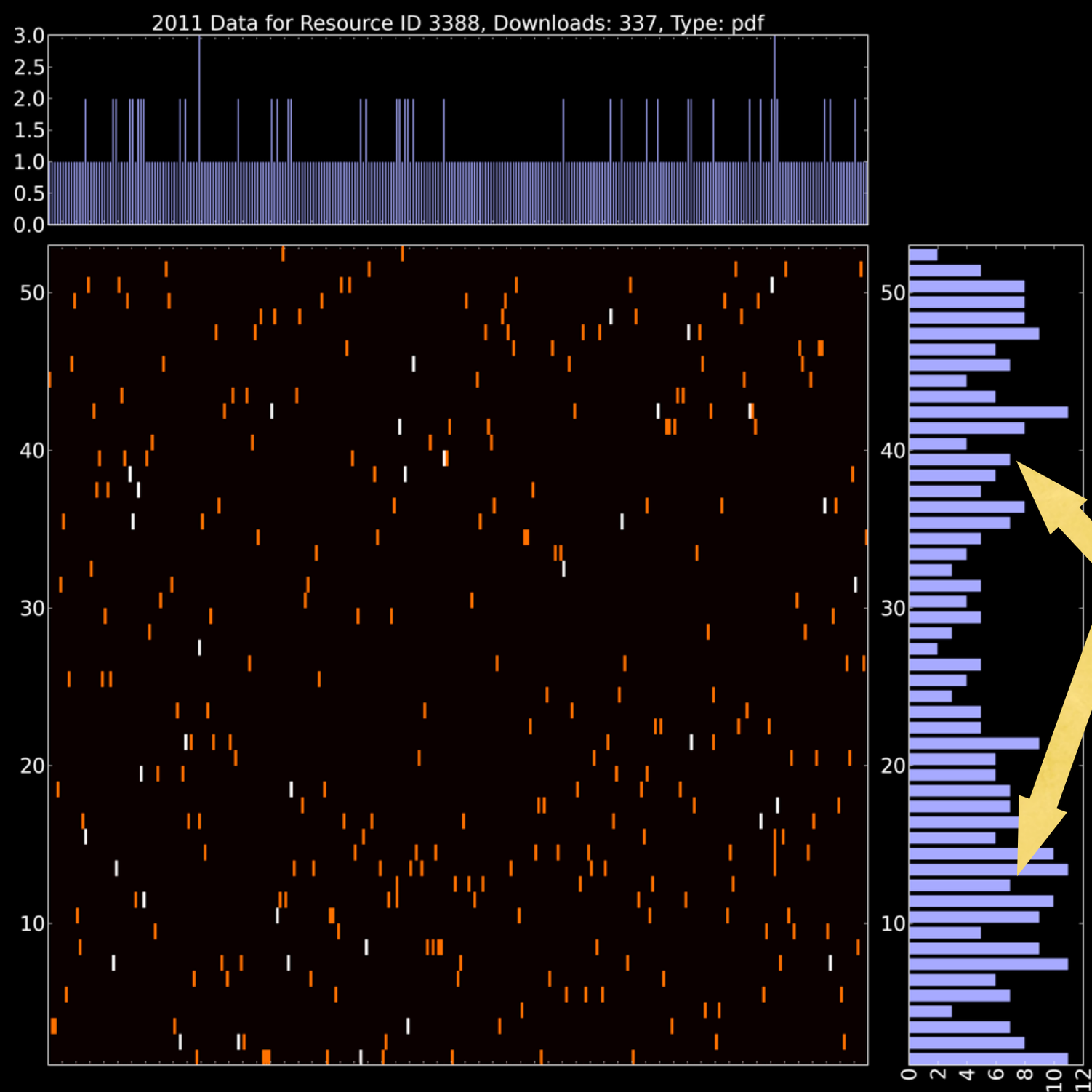


2:Visualization



Intensity of color = number of downloads from a given IP during a given week

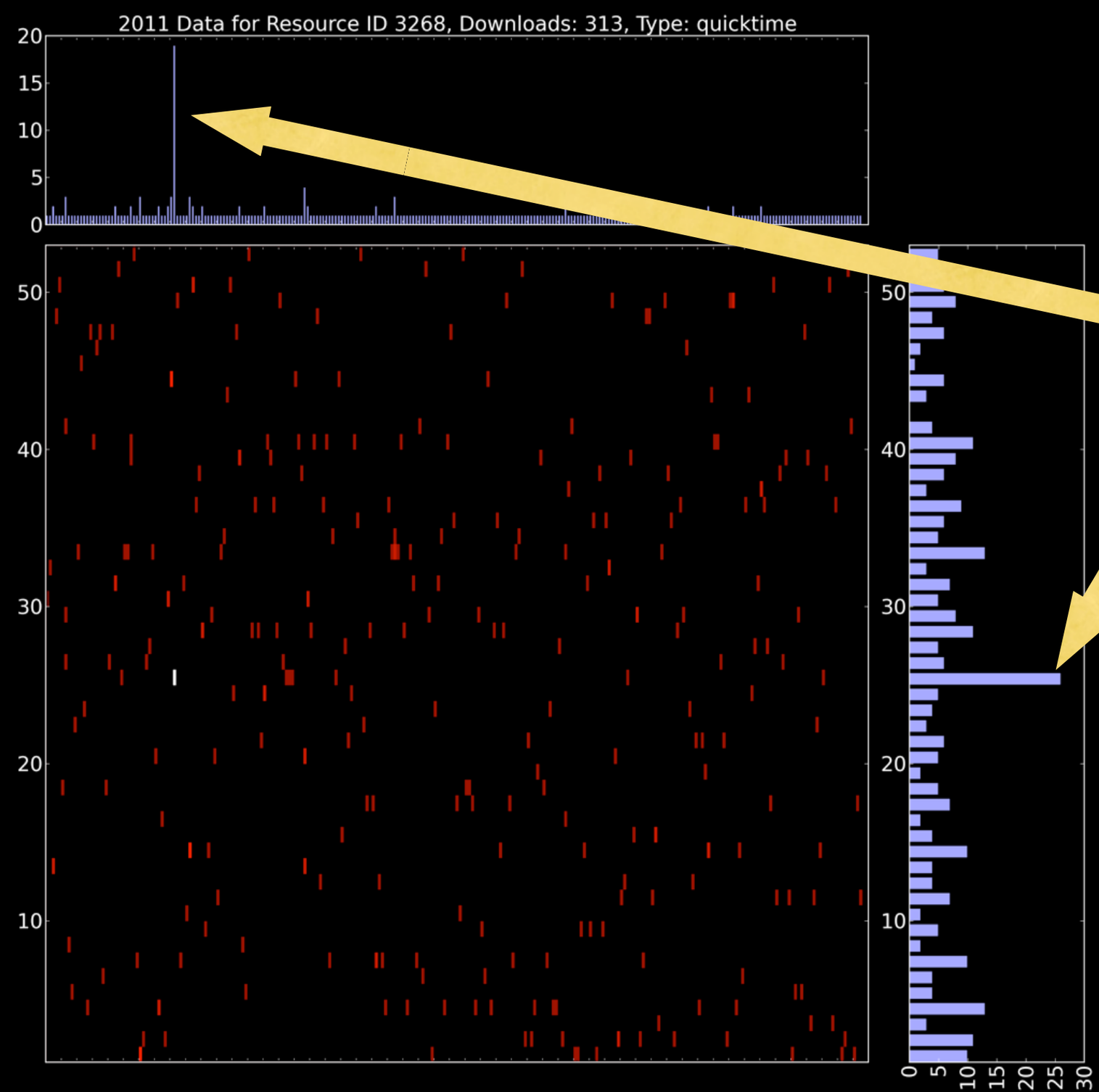
2:Visualization



Many Locations

Seasonal

2:Visualization

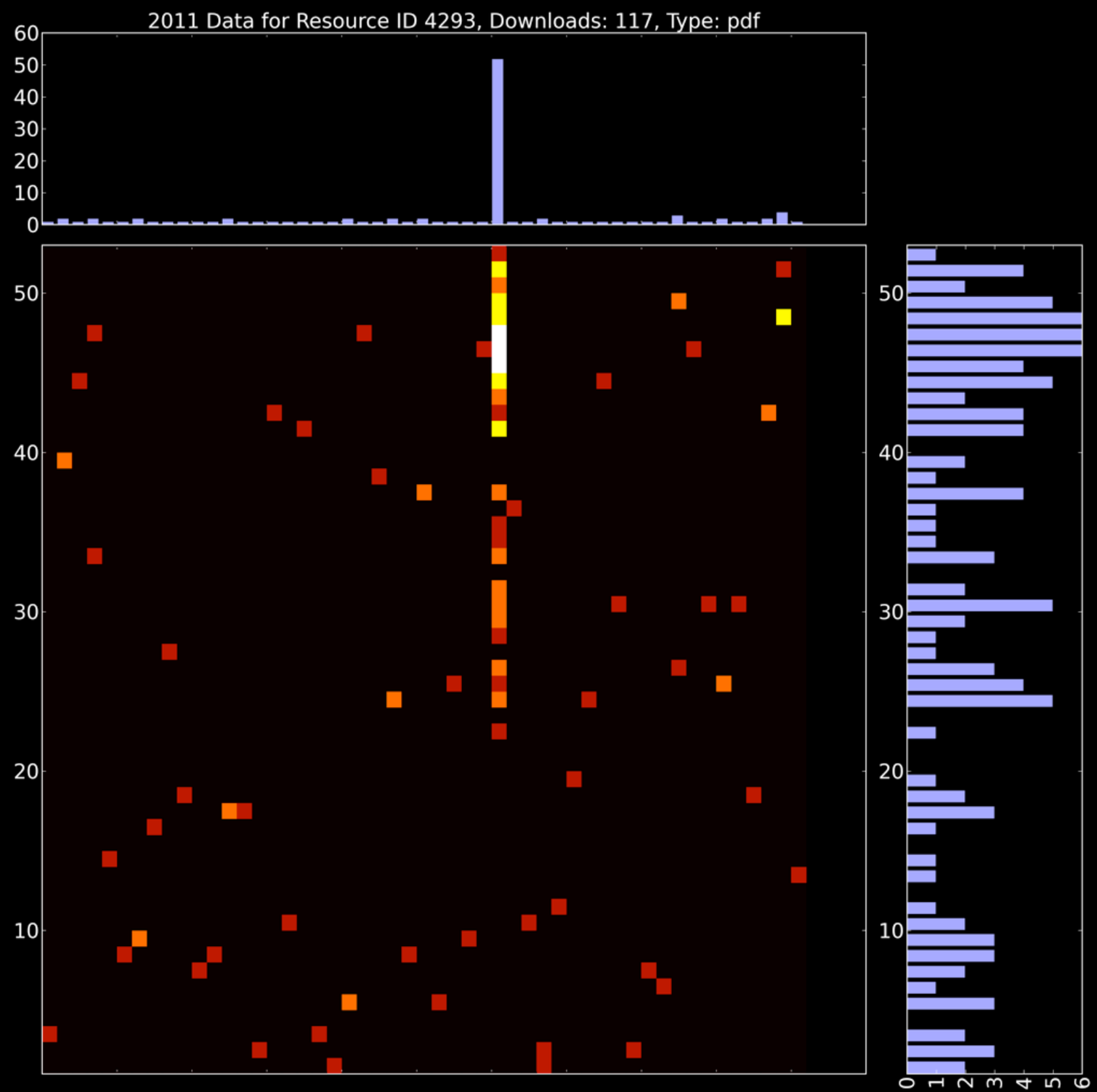


Single Main Location

Event Based

Many Minor Locations

2:Visualization

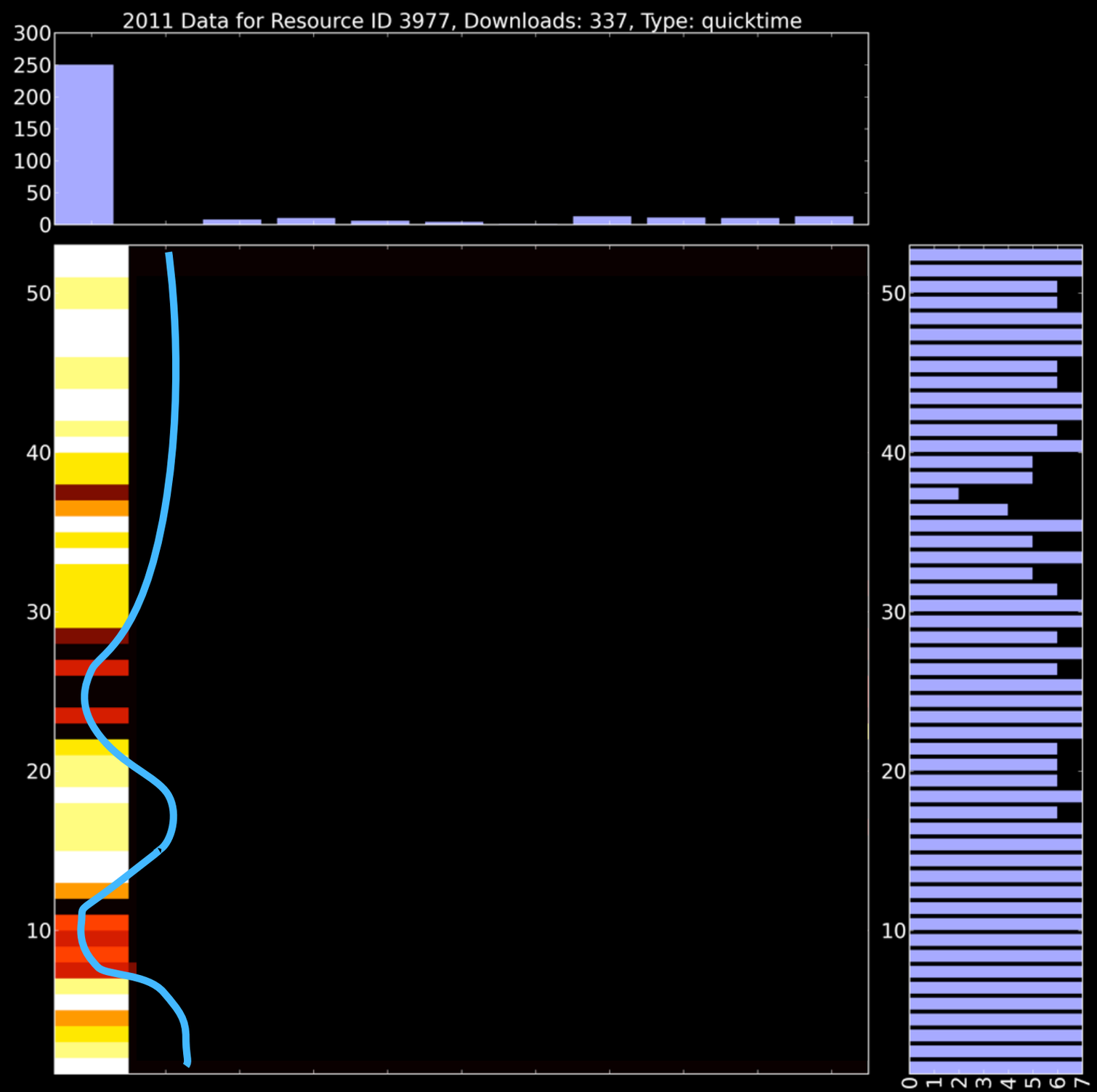


Even Access

+

Adoption in Fall at Single Location

2:Visualization



Seasonal Access from One Location

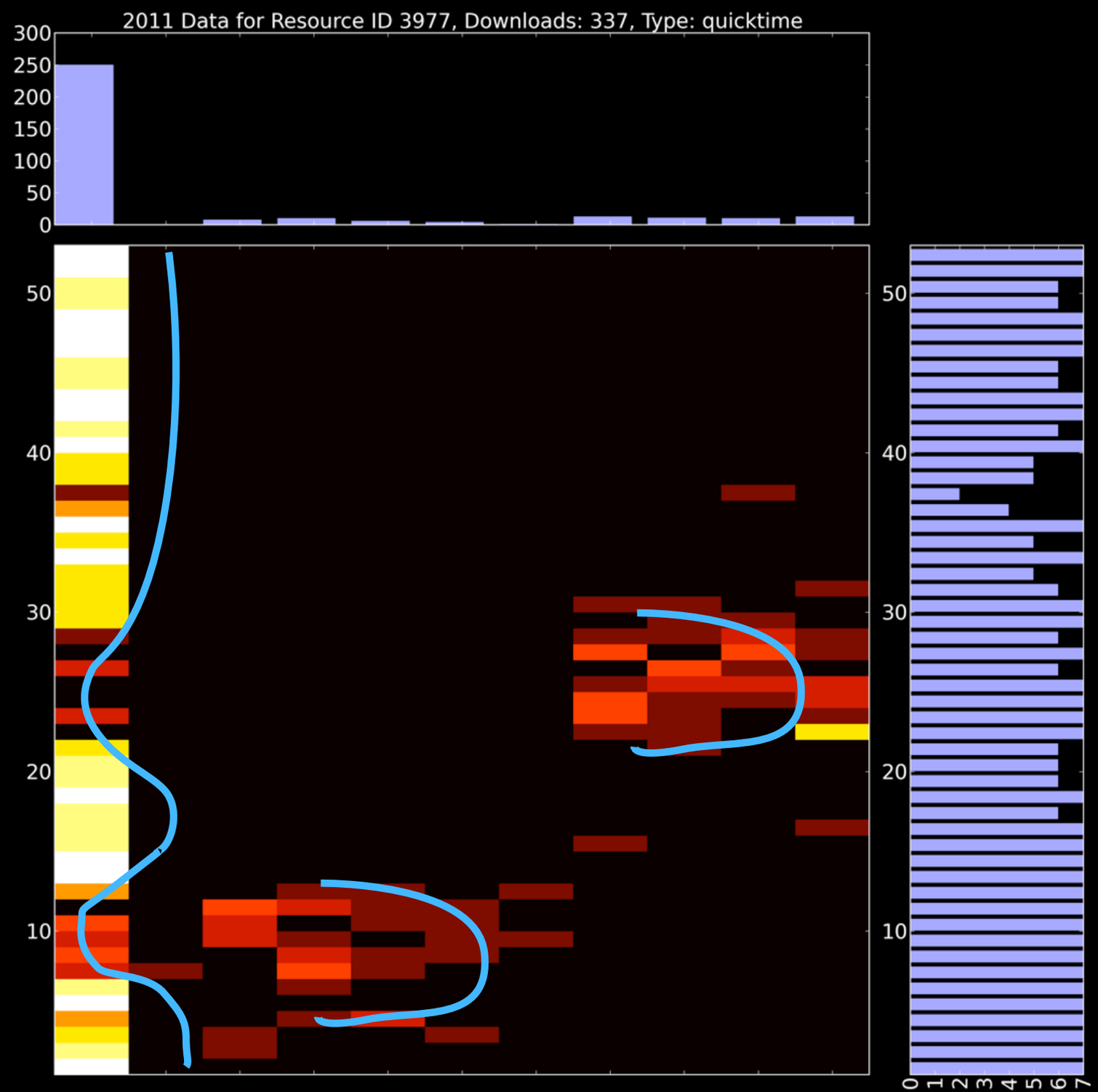
+

Clustered Access from Two Locations

=

Level Access

2:Visualization



Seasonal Access from One Location

+

Clustered Access from Two Locations

=

Level Access

3: Parameter Space Exploration

Quantum Dot Lab | Terminate | Keep for later

1 Input → 2 Simulate

About this tool
Questions?

Number of States: 7

Surface passivation: ☑ yes

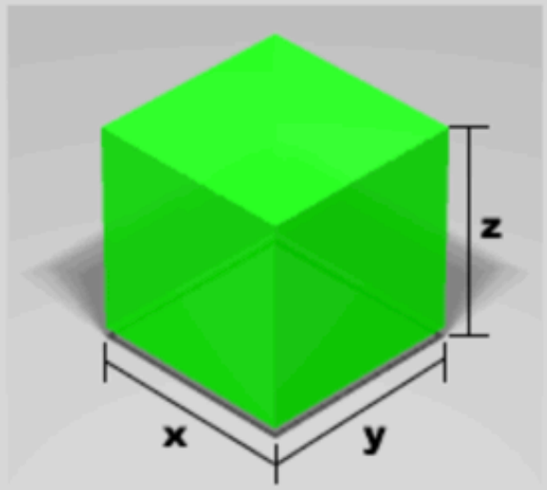
Device Structure | Light Source

Geometry: Cuboid

X dimensions: 5nm

Y dimensions: 5.5nm

Z dimensions: 6nm



Effective Mass: 0.067

Discretization: 0.565nm

Energy gap: 1.43eV

3: Parameter Space Exploration

Quantum Dot Lab

1 Input → 2 Simulate

Number of States: 7

Surface passivation: yes

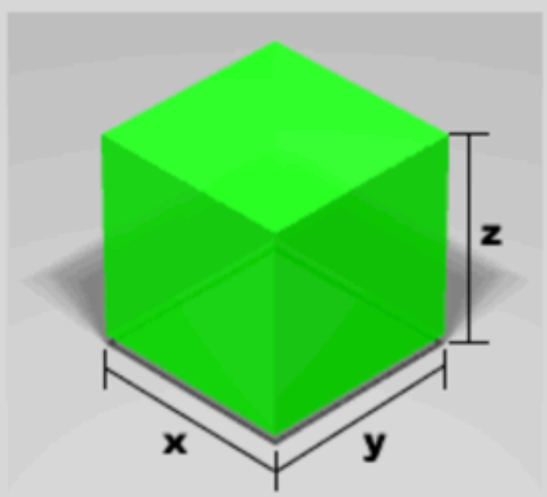
Device Structure | Light Source

Geometry: Cuboid

X dimensions: 5nm

Y dimensions: 5.5nm

Z dimensions: 6nm



Effective Mass: 0.067

Discretization: 0.565nm

Energy gap: 1.43eV

Number of States: 7

Surface passivation: yes

Device Structure | Light Source

Geometry: Cuboid

X dimensions: 5nm

Y dimensions: 5.5nm

Z dimensions: 6nm

Effective Mass: 0.067

Discretization: 0.565nm

Energy gap: 1.43eV

3: Parameter Space Exploration

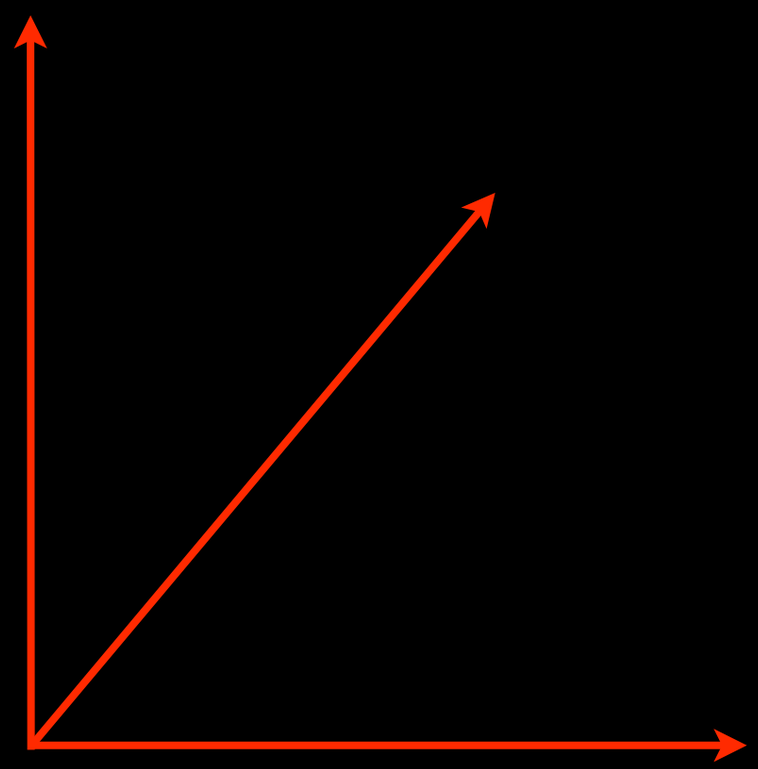
- Can we go one level deeper into tool analysis by looking at how users parameterize their simulations?
- Are there patterns?
- Will these patterns help us learn how to guide users based on the experience of others?
- Will these patterns help us make user-user social introductions of scientific merit?

3: Parameter Space Exploration

- Many tools have more than 10 parametric dimensions

- Some have in excess of 30

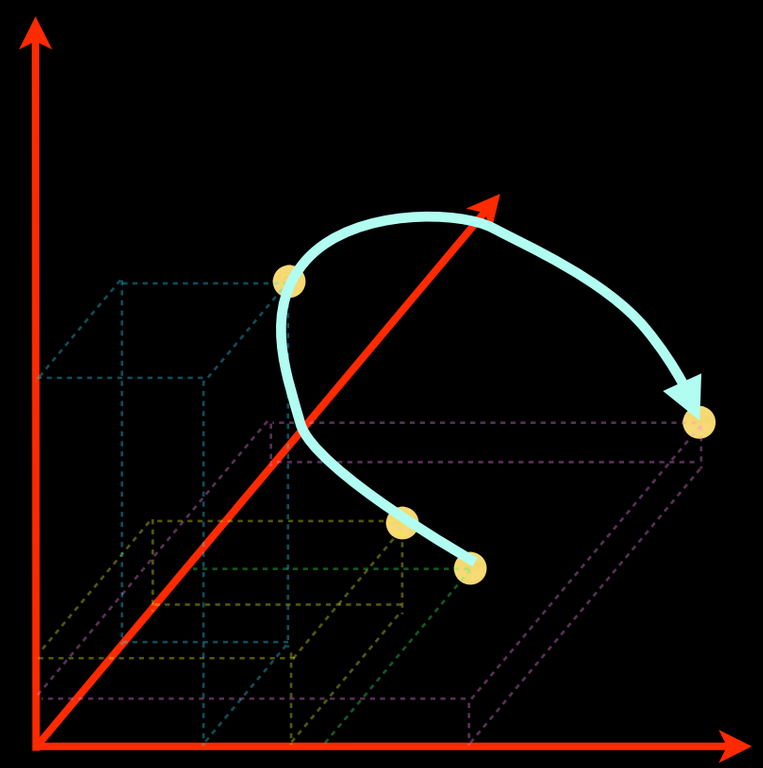
3: Parameter Space Exploration



X dimensions:	5nm
Y dimensions:	5.5nm
Z dimensions:	6nm

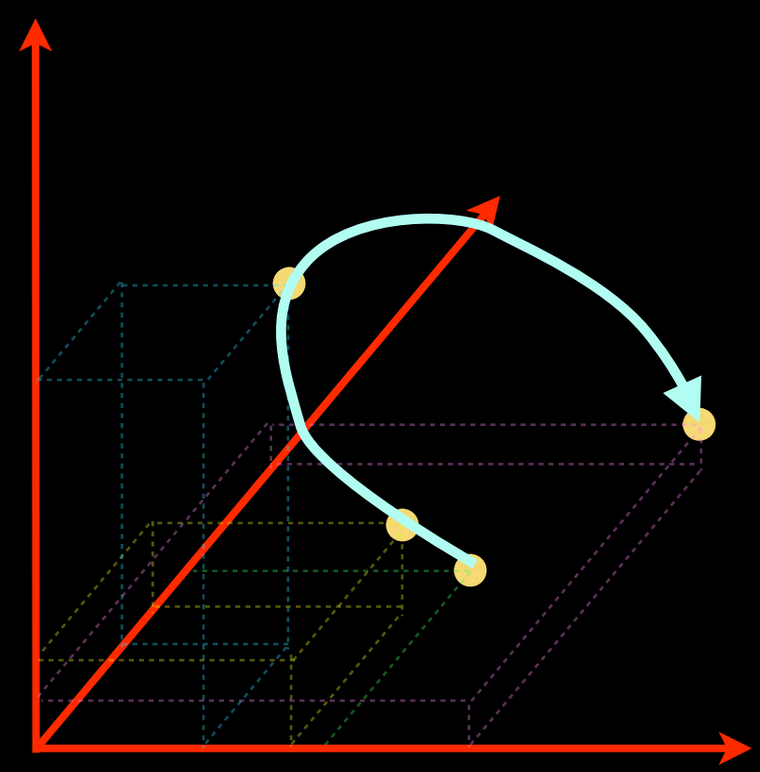
3: Parameter Space Exploration

In general, how do we represent a path through n-dimensional parameter space in 2 dimensions?



X dimensions:	5nm
Y dimensions:	5.5nm
Z dimensions:	6nm

3: Parameter Space Exploration



In general, how do we represent a path through n-dimensional parameter space in 2 dimensions?

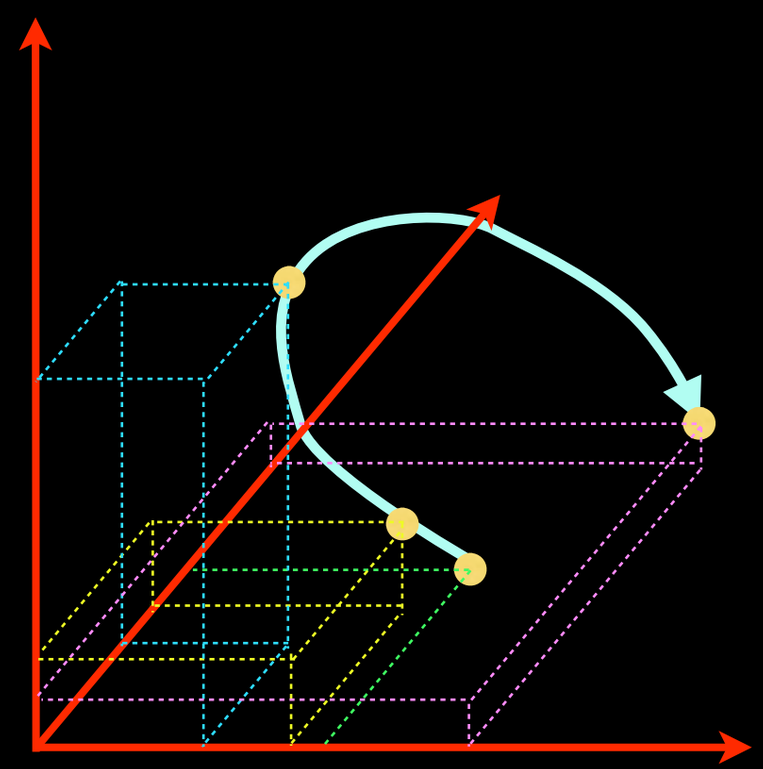
	X	Y	Z
Point 1	2	2	0
Point 2	1.8	0.7	0.6
Point 3	1.1	2.5	1.1
Point 4	3.8	0.4	3.7

$$\sqrt{(X_1-X_2)^2+(Y_1-Y_2)^2+(Z_1-Z_2)^2}$$

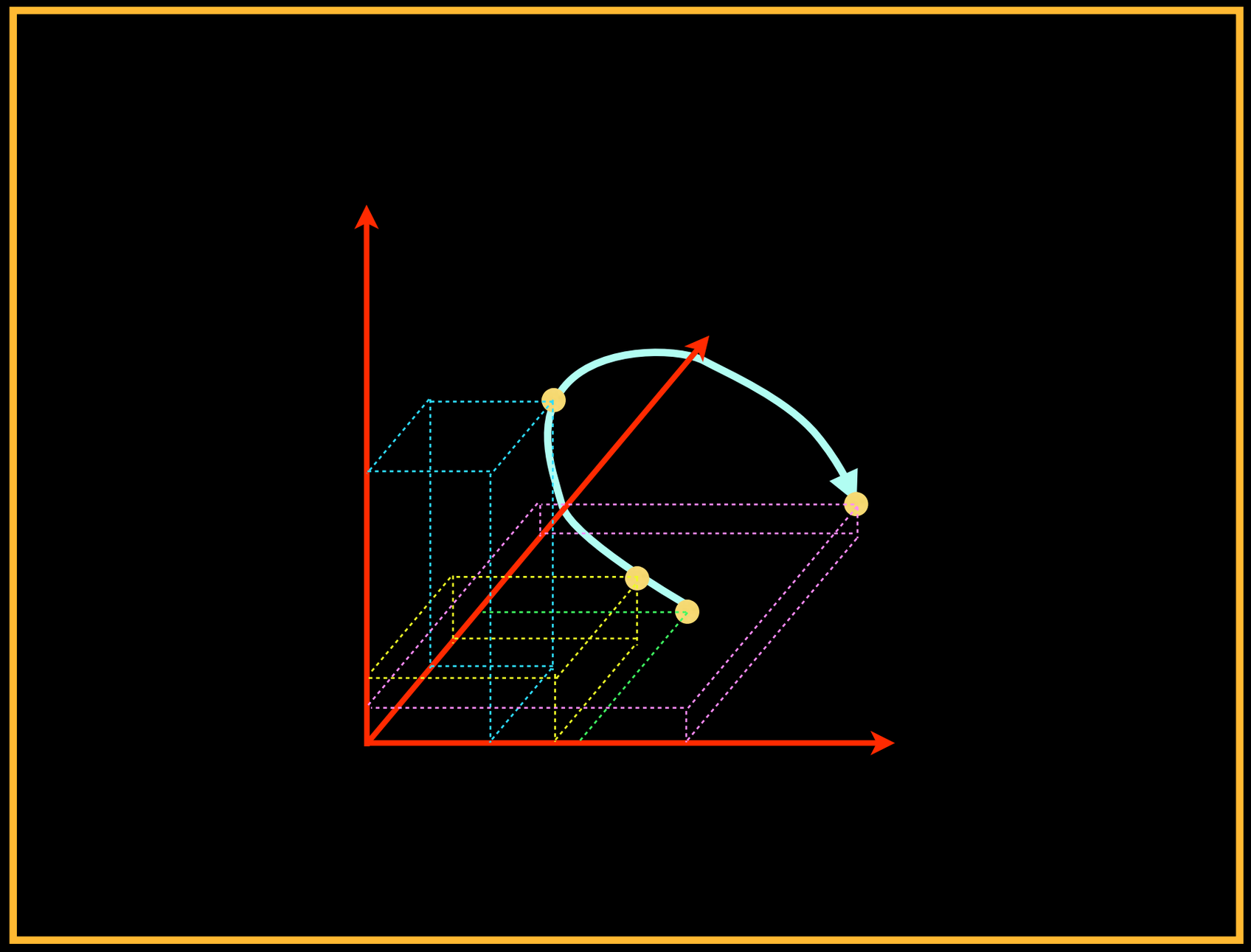
X dimensions:	5nm
Y dimensions:	5.5nm
Z dimensions:	6nm

	Point 1	Point 2	Point 3	Point 4
Point 1	0.00	1.45	1.51	4.41
Point 2	1.45	0.00	1.99	3.70
Point 3	1.51	1.99	0.00	4.30
Point 4	4.41	3.70	4.30	0.00

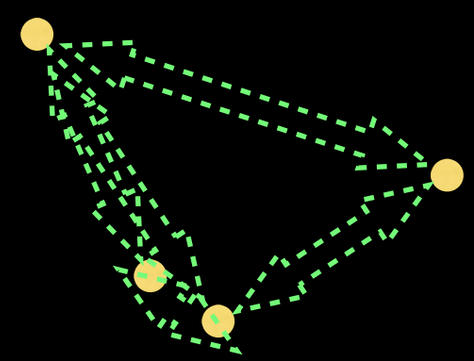
3: Parameter Space Exploration



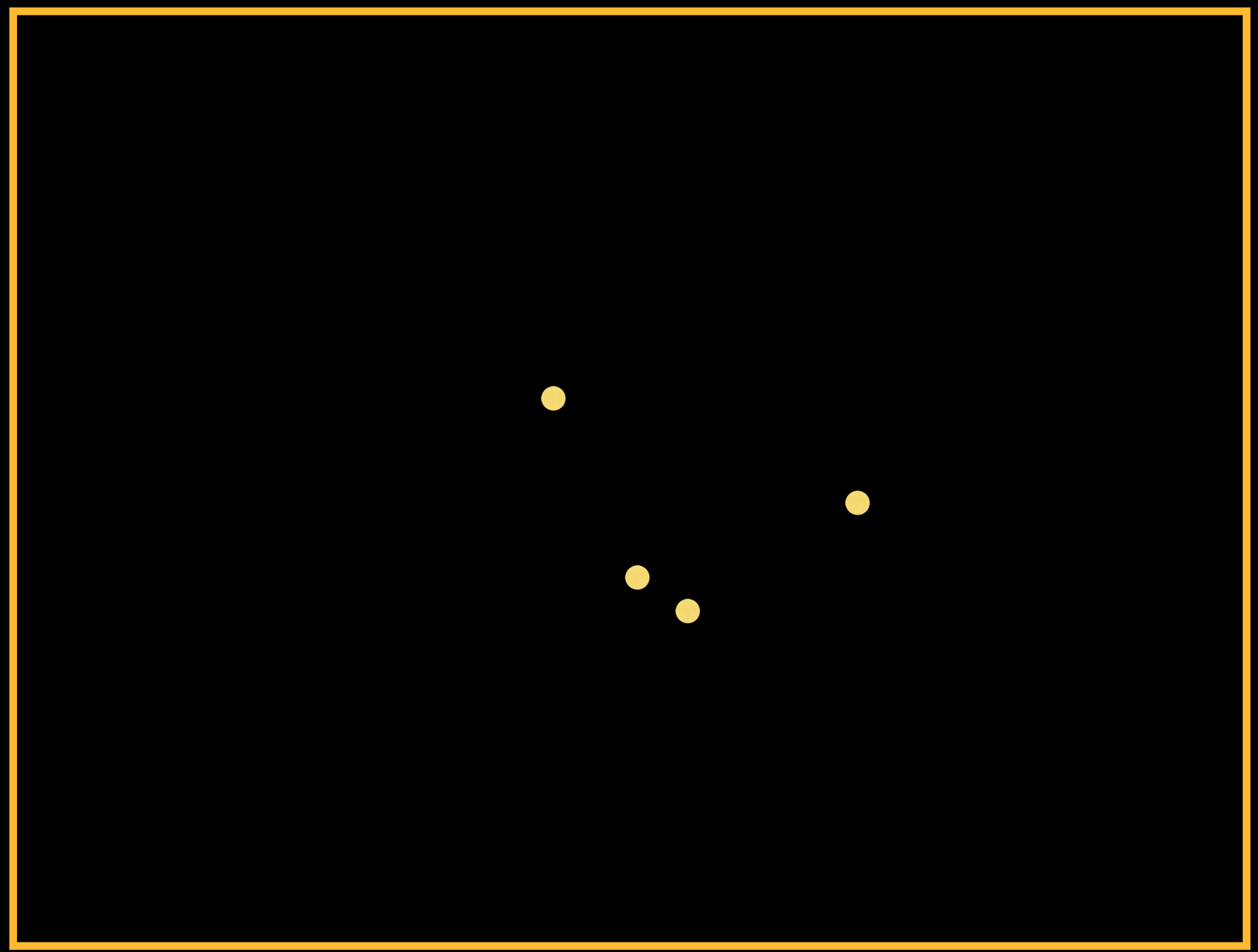
3: Parameter Space Exploration



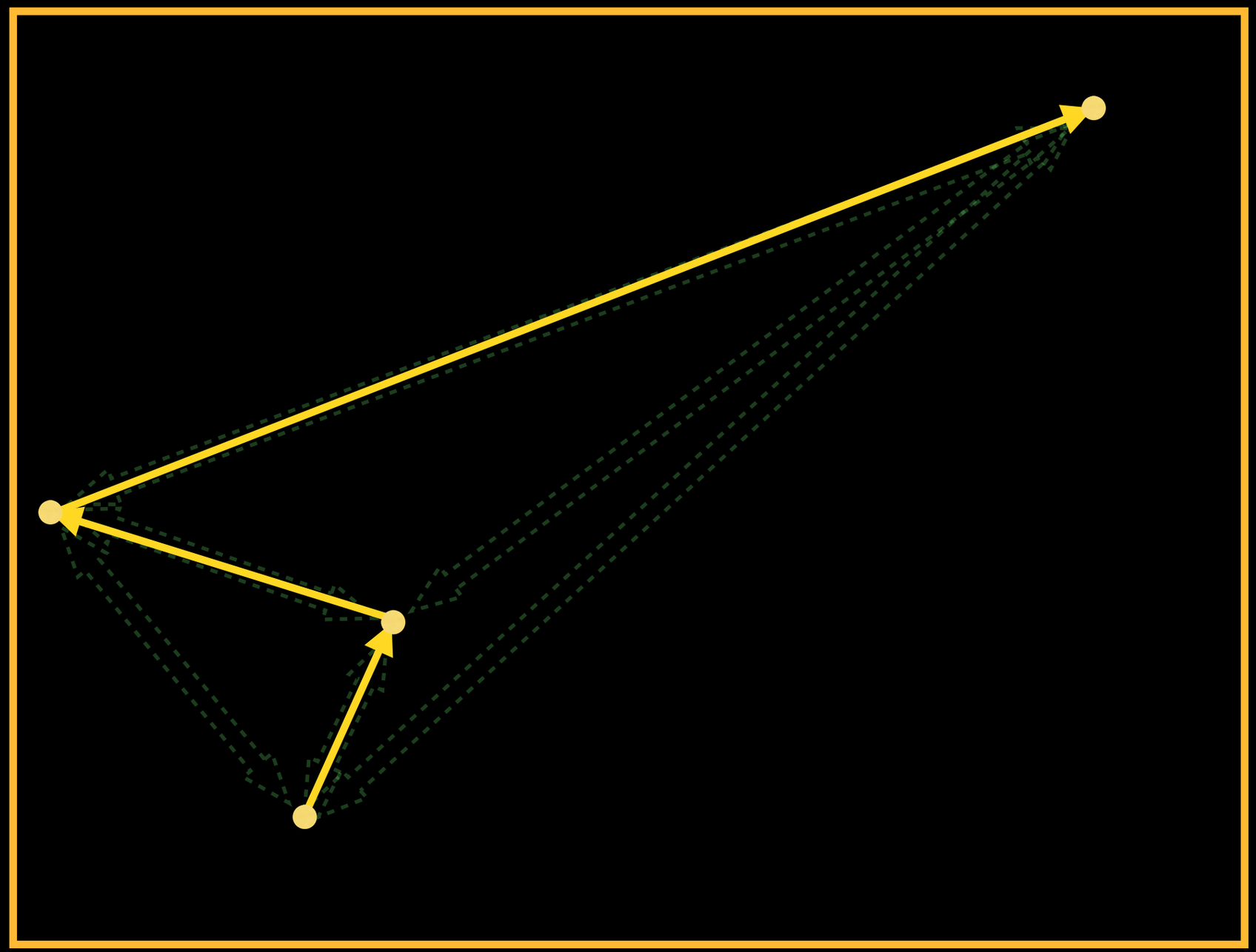
3: Parameter Space Exploration



3: Parameter Space Exploration



3: Parameter Space Exploration



3: Parameter Space Exploration

- Size of ball ~ number of parameters changed
- Color of ball ~ a subset of parameters

3: Parameter Space Exploration

- Size of ball ~ number of parameters changed
- Color of ball ~ a subset of parameters
  - ΔX
  - ΔY
  - ΔZ

3: Parameter Space Exploration

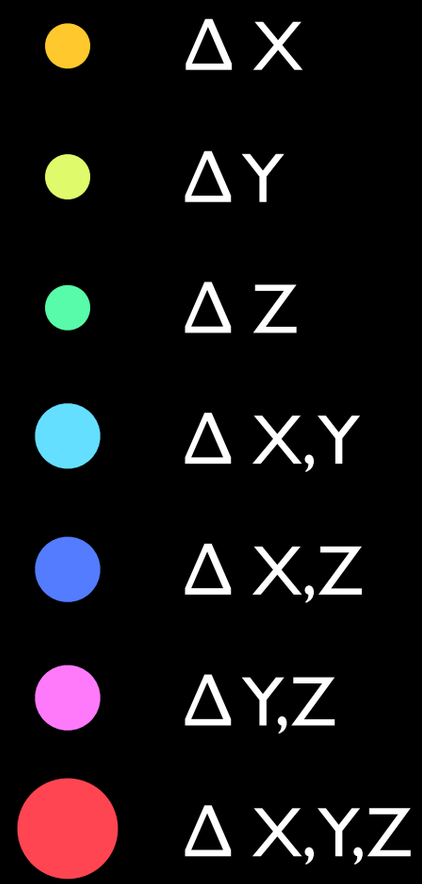
- Size of ball ~ number of parameters changed
- Color of ball ~ a subset of parameters
  - Δ X
  - Δ Y
  - Δ Z
  - Δ X,Y
  - Δ X,Z
  - Δ Y,Z

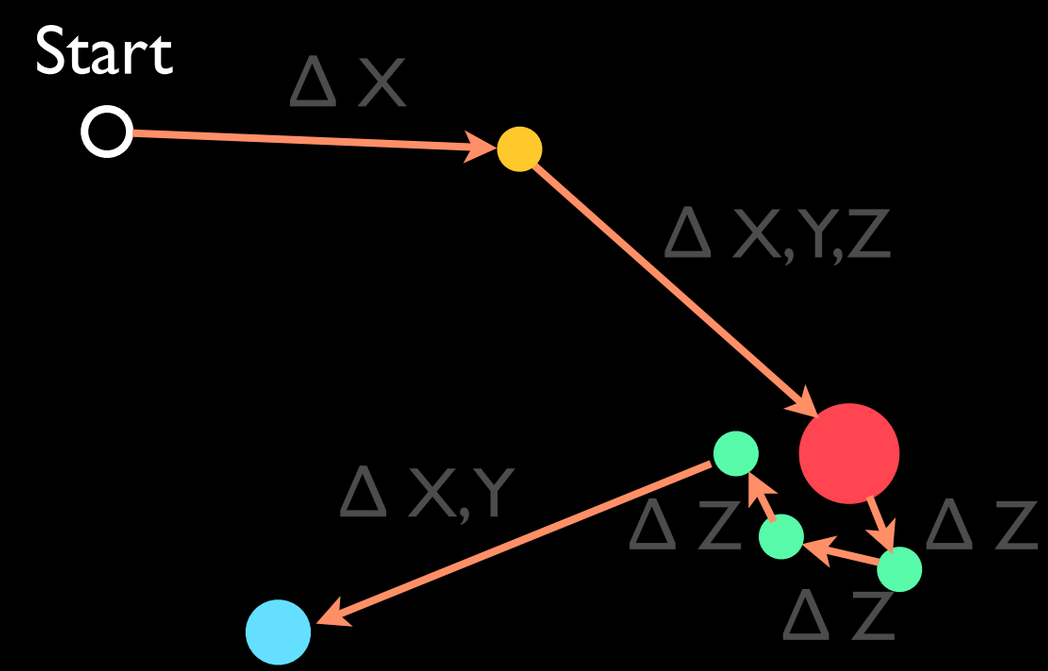
3: Parameter Space Exploration

- Size of ball ~ number of parameters changed
- Color of ball ~ a subset of parameters
  - Δ X
  - Δ Y
  - Δ Z
  - Δ X,Y
  - Δ X,Z
  - Δ Y,Z
  - Δ X,Y,Z

3: Parameter Space Exploration

- Size of ball ~ number of parameters changed
- Color of ball ~ a subset of parameters





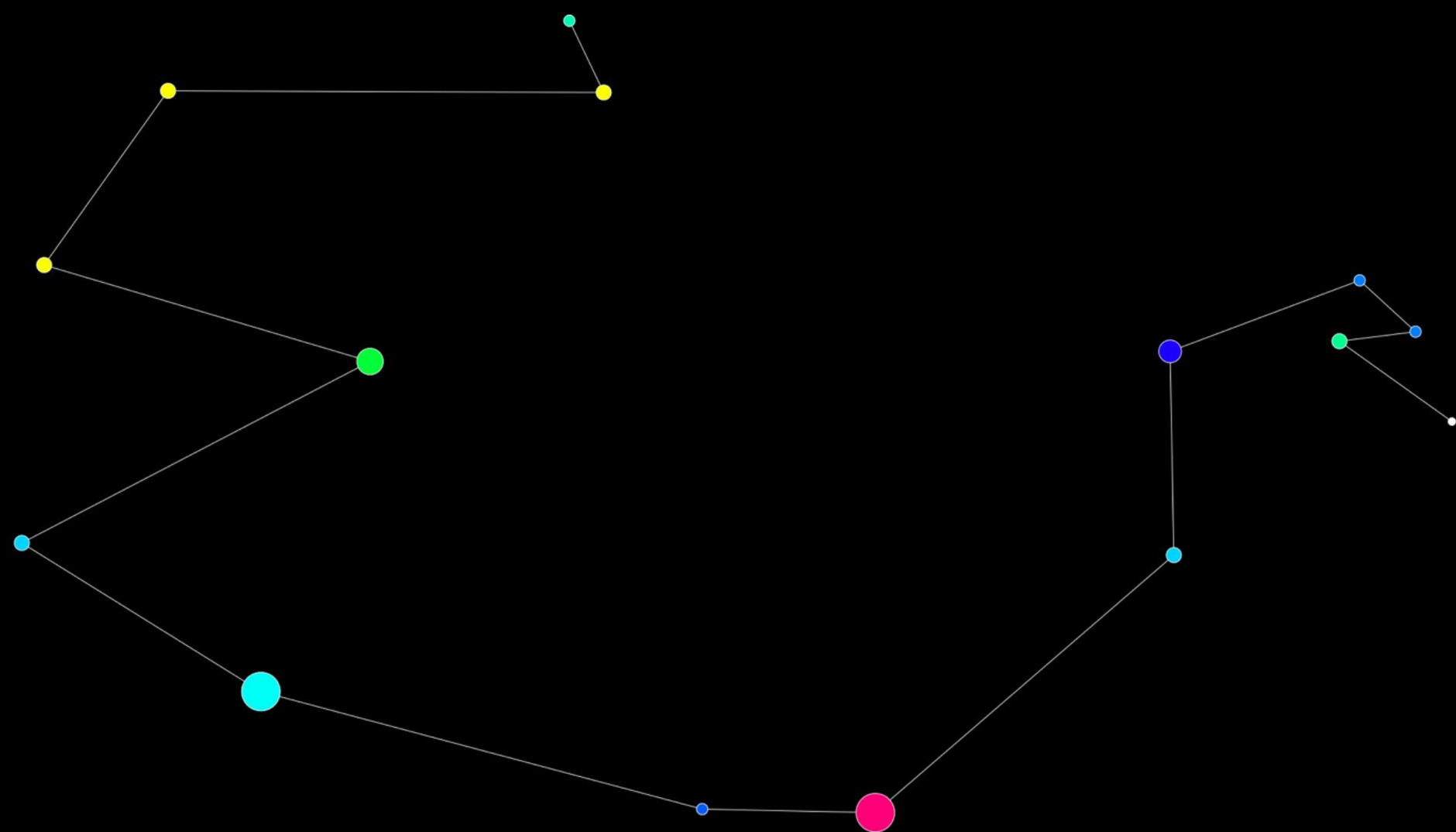
3: Parameter Space Exploration

Hypotheses on Exploration Behavior:

- Wanderers
- Searchers
- Surveyors
- Wildcatters
- Permuters
- others?

3: Parameter Space Exploration

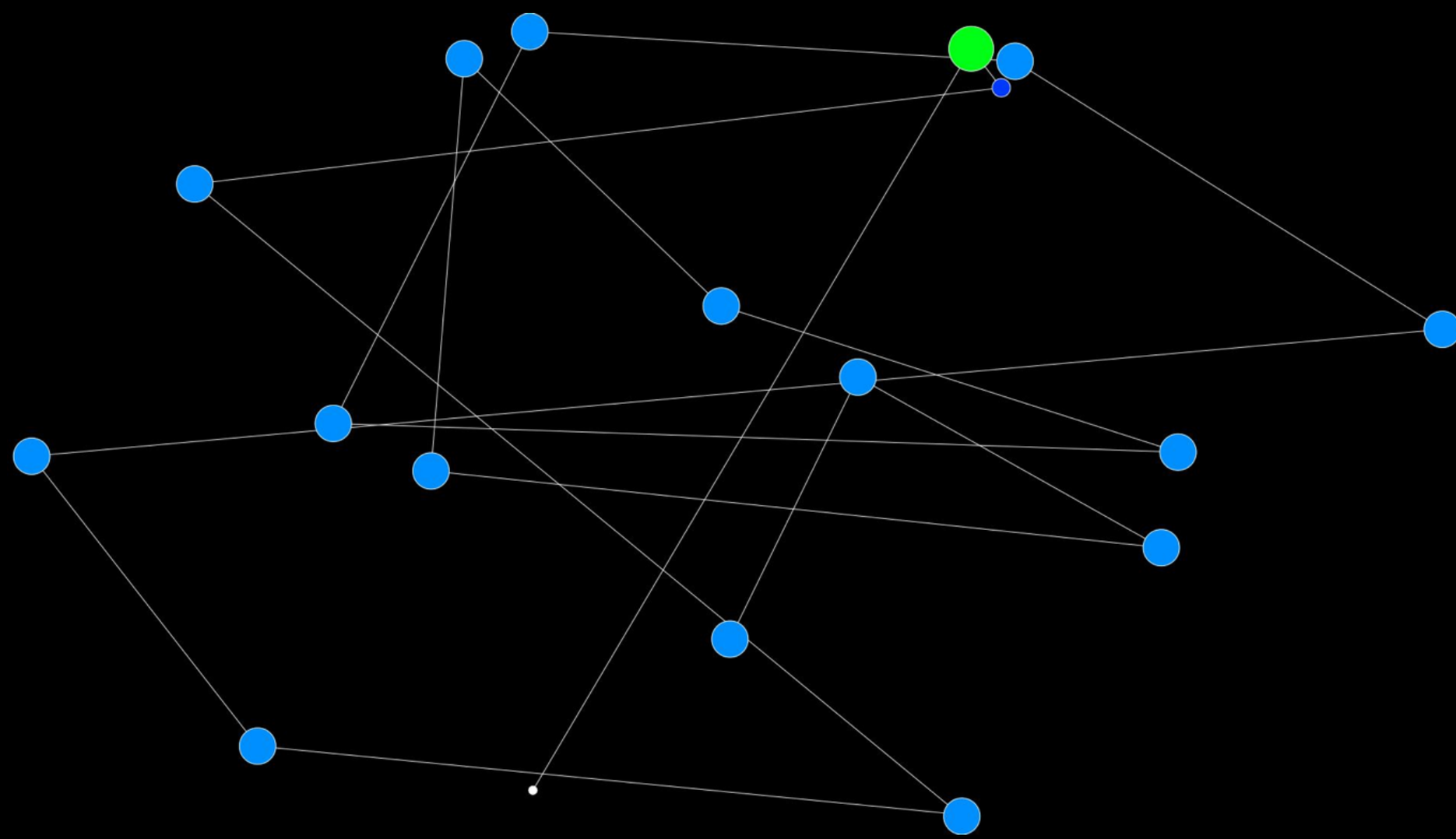
"*wanderer*" - walks extensively, changes different parameters



Example user sessions with tool "pntoy"

3: Parameter Space Exploration

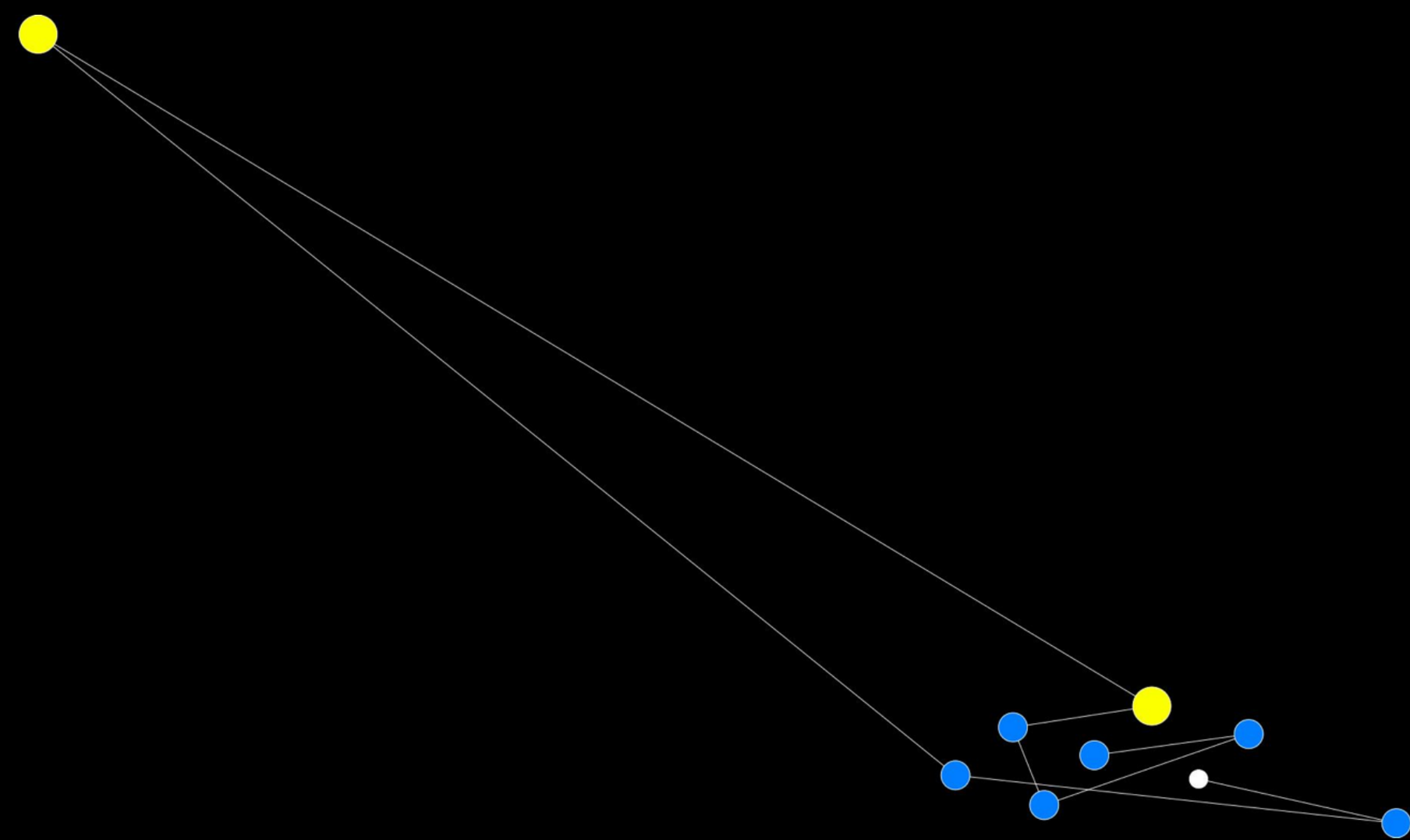
"*wildcatter*" - walks extensively, changes same parameters



Example user sessions with tool "pntoy"

3: Parameter Space Exploration

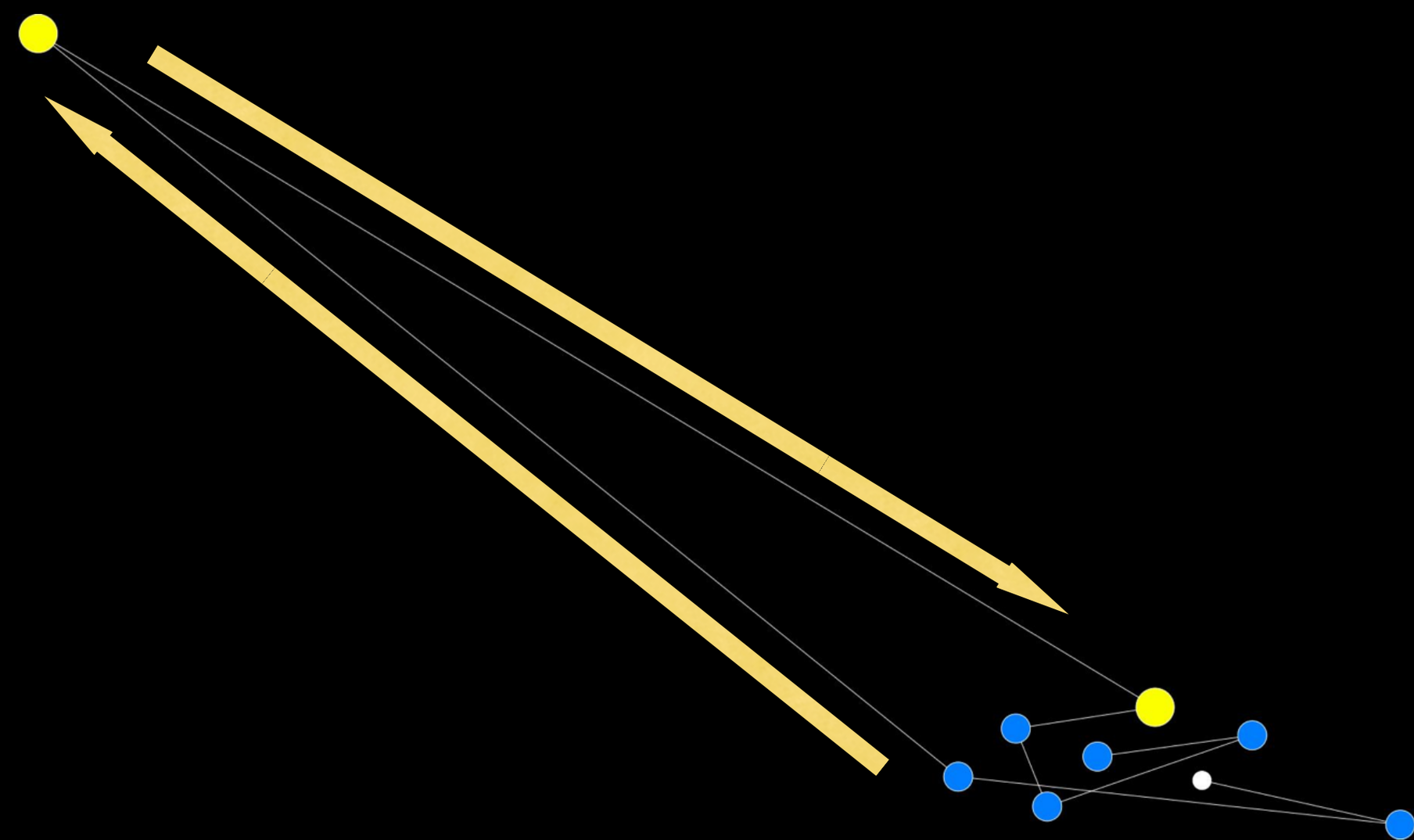
"*searcher*" - focused walk, similar parameters,
one experimental deviation with a quick return



Example user sessions with tool "pntoy"

3: Parameter Space Exploration

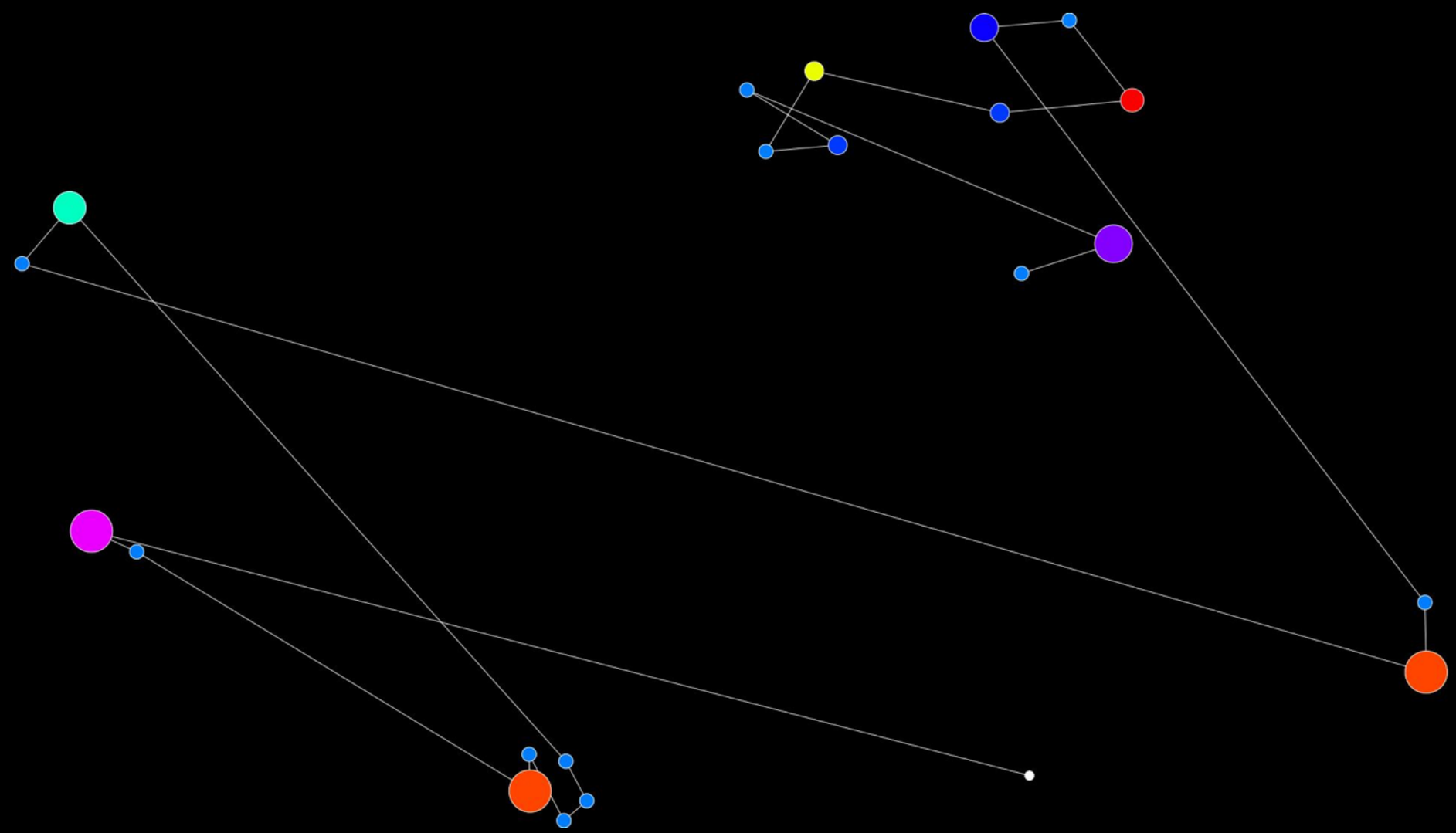
"*searcher*" - focused walk, similar parameters,
one experimental deviation with a quick return



Example user sessions with tool "pntoy"

3: Parameter Space Exploration

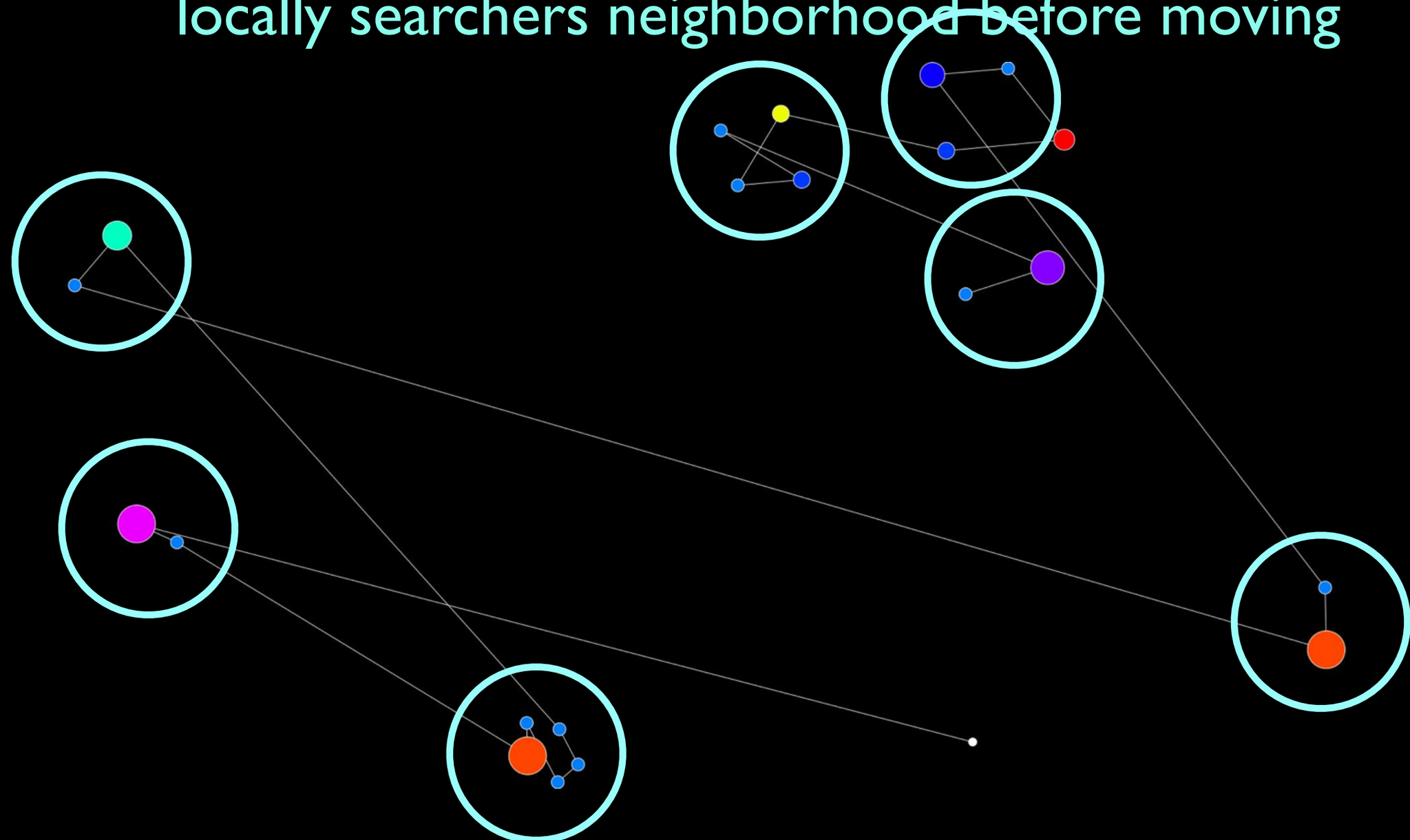
"*surveyor*" - extensive walk, similar parameters,
locally searchers neighborhood before moving



Example user sessions with tool "pntoy"

3: Parameter Space Exploration

"*surveyor*" - extensive walk, similar parameters,
locally searchers neighborhood before moving



Example user sessions with tool "pntoy"

What Are We Answering & Why?

Past

➥ What have users done?
What impact have we had?

Present

Future

What Are We Answering & Why?

Past

➥ What have users done?
What impact have we had?

Present

➥ How can we use that information to:
Guide our users?
Allocate resources?

Future

What Are We Answering & Why?

Past

➥ What have users done?
What impact have we had?

Present

➥ How can we use that information to:
Guide our users?
Allocate resources?

Future

➥ How can we:
Plan for our users' needs?
Increase our value & impact?

Serve a Changing User Perspective

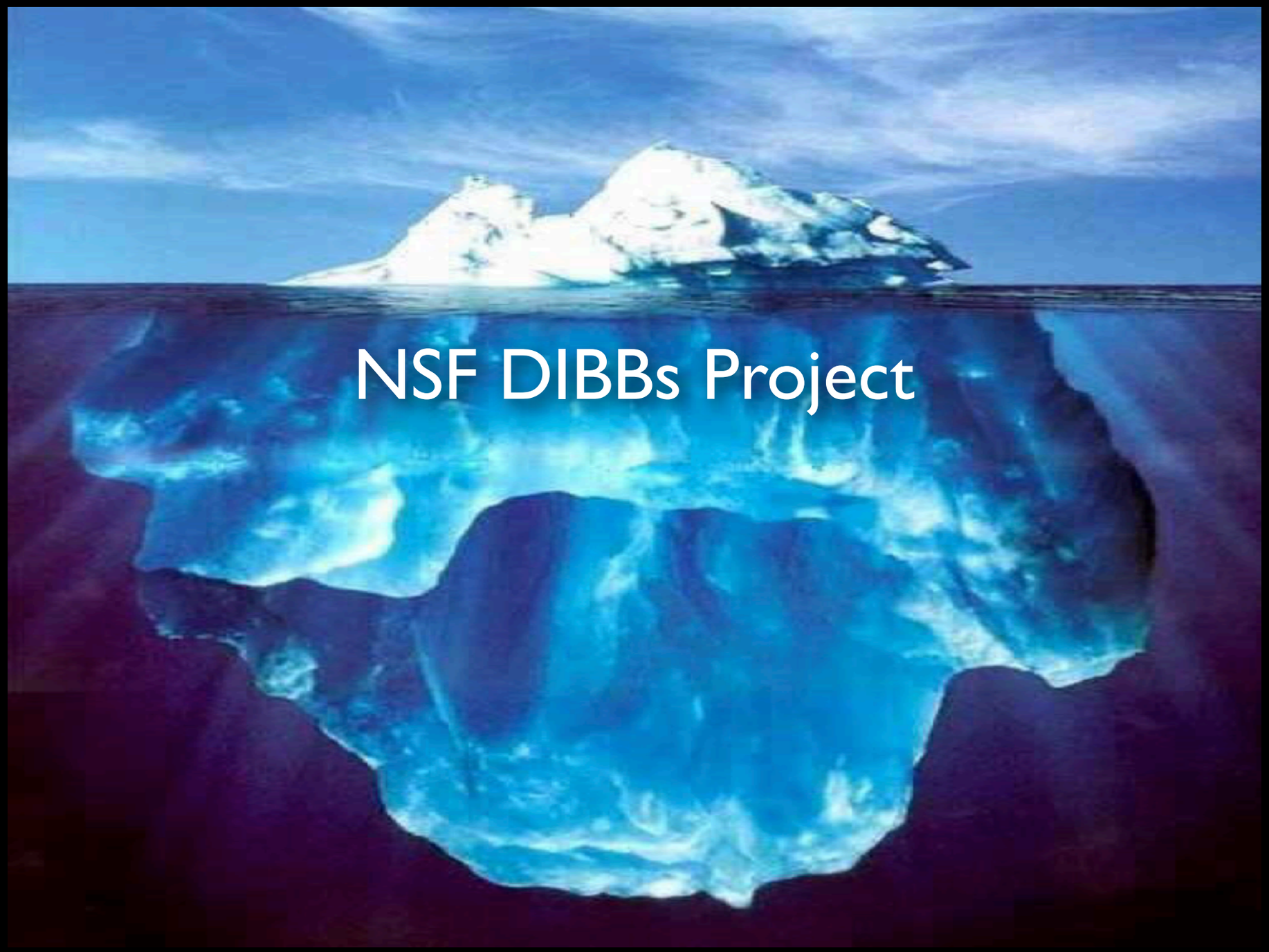
Past ➥ What can I acquire?

Present ➥ What should I do?

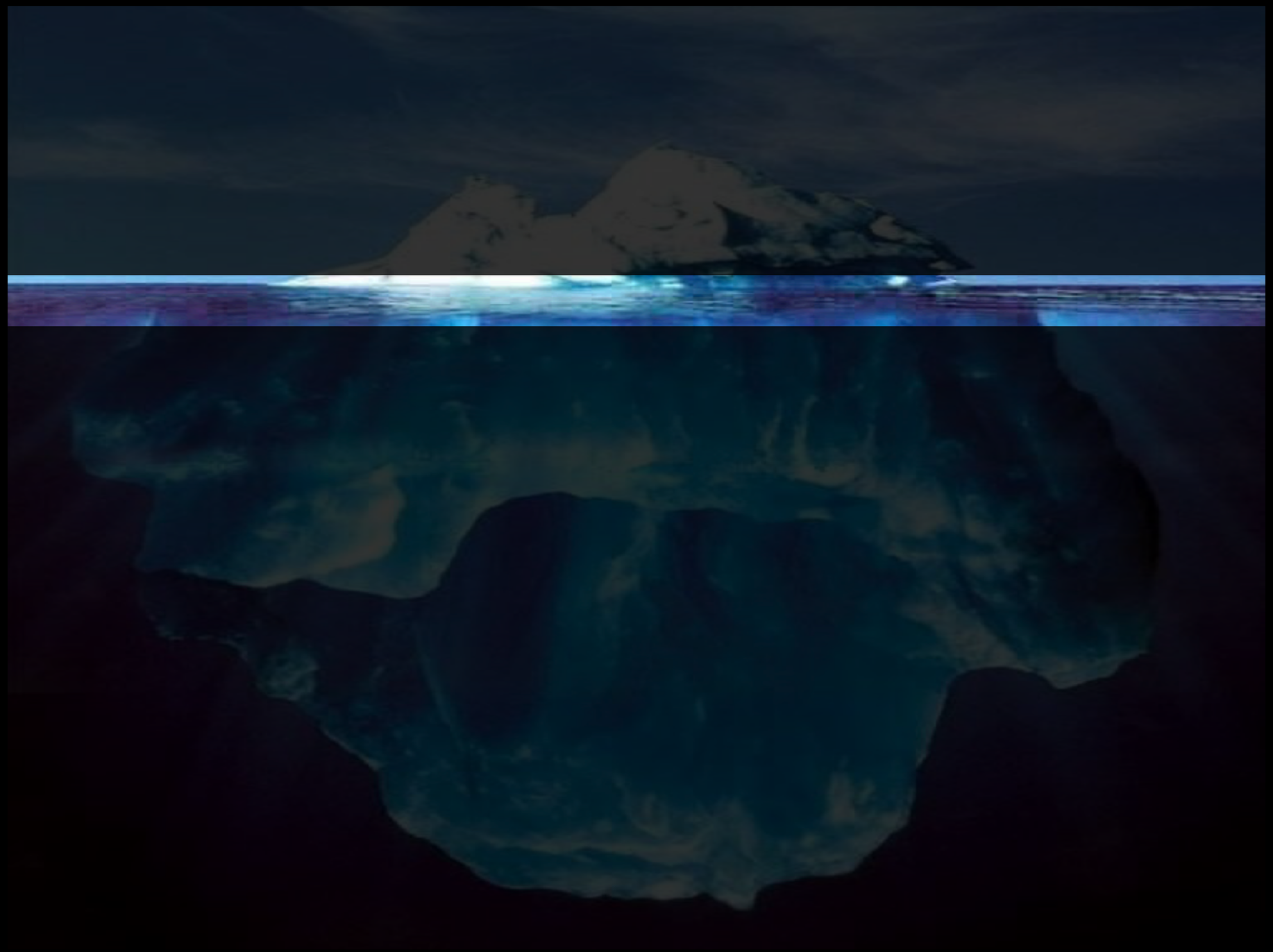
Future ➥ What can I accomplish?

Savanna to...

...Arctic



Ocean Surface = Data



Above = Query Tools

Simulation Tools

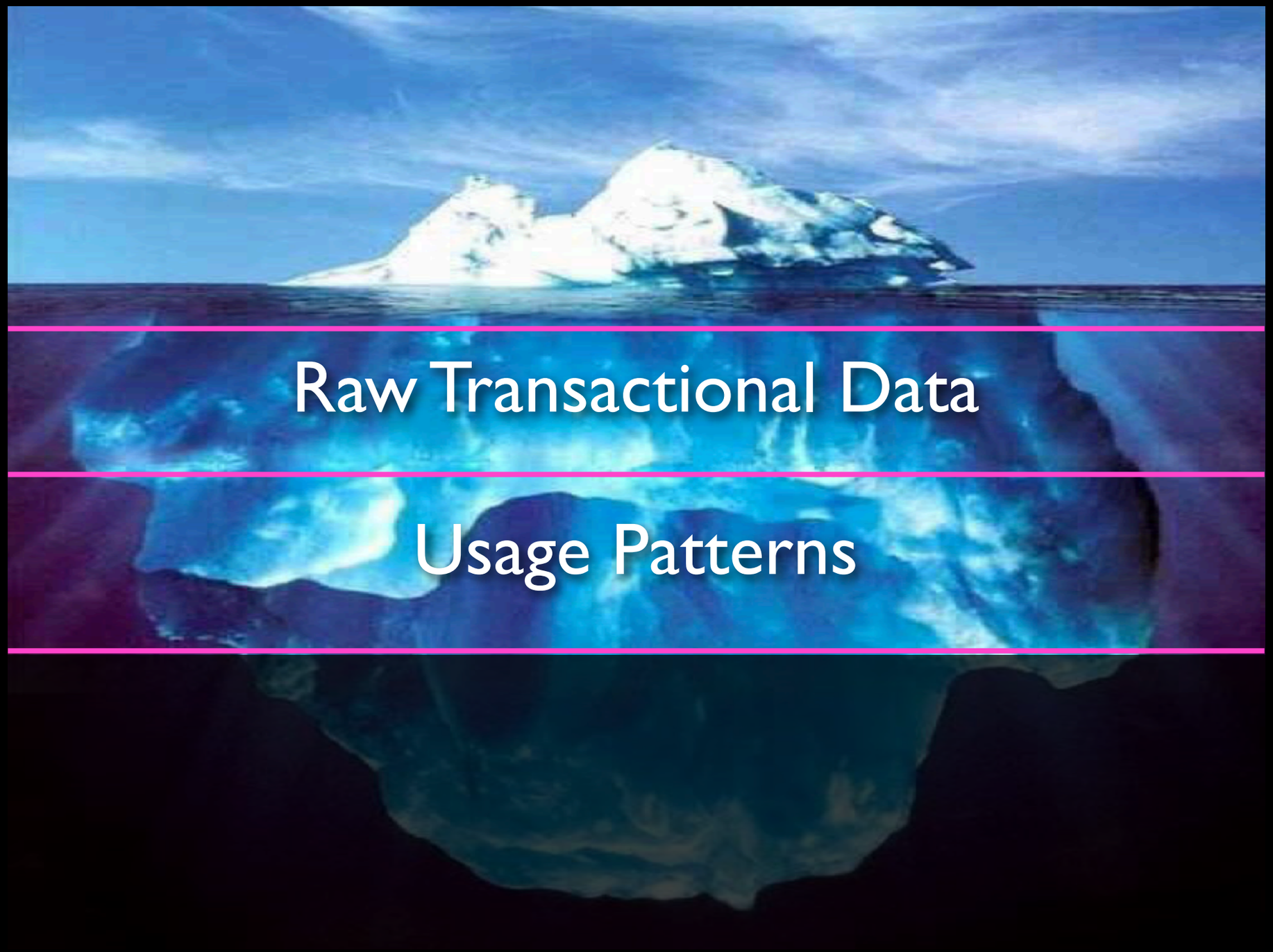
SQL

Data Exploration Interfaces

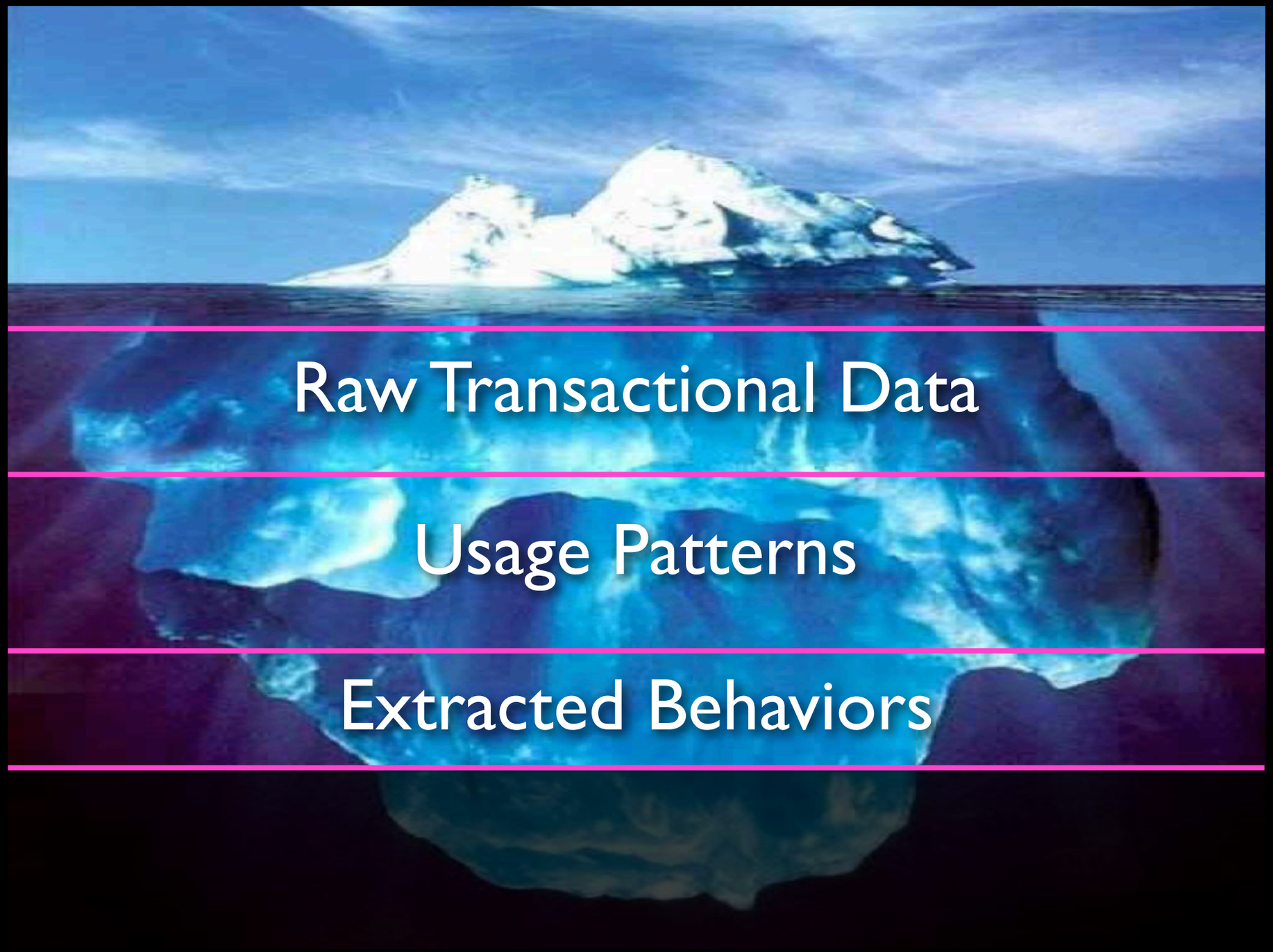
Reporting Tools

Below = Data Use Data

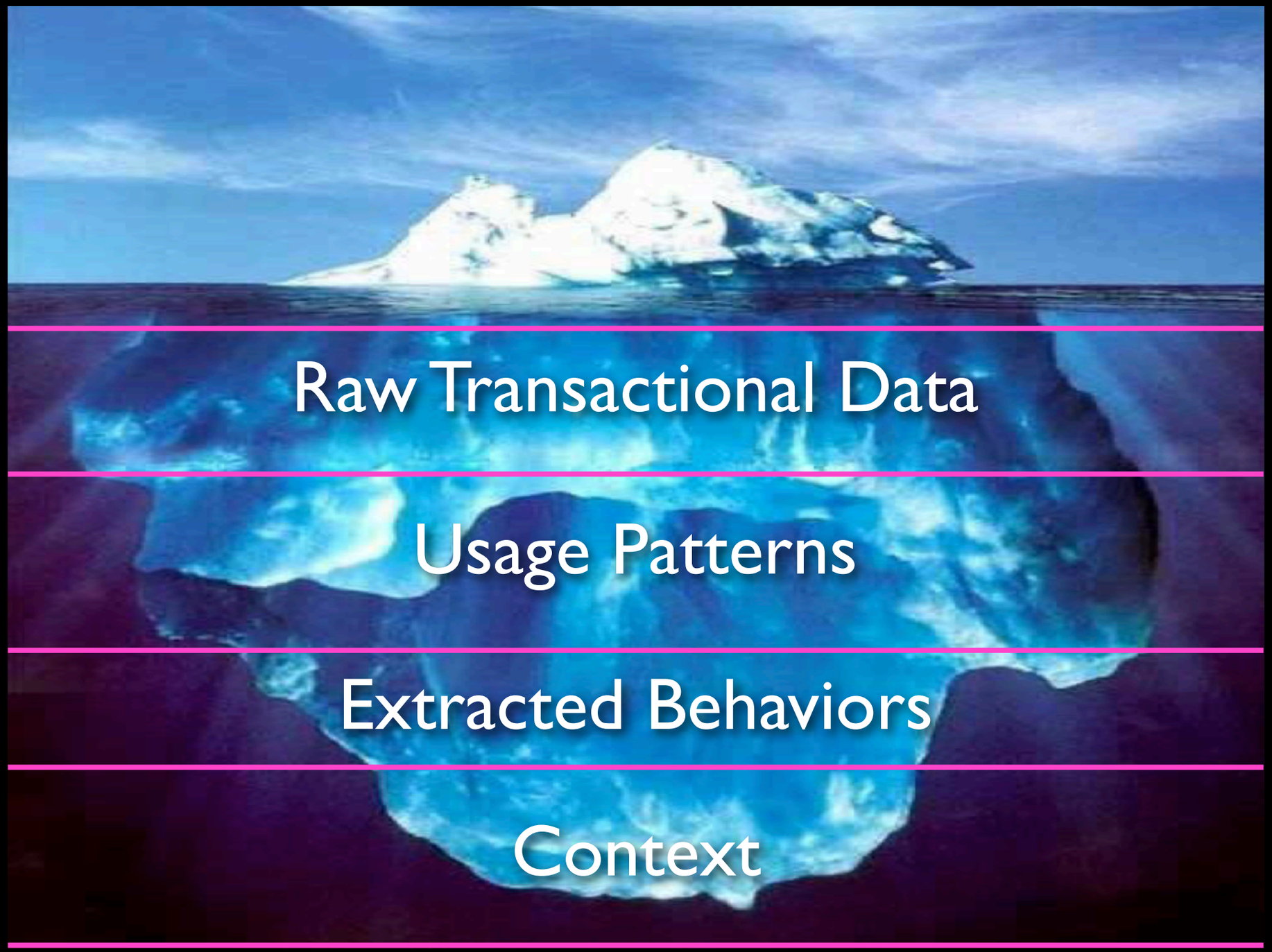
Below = Data Use Data



Below = Data Use Data

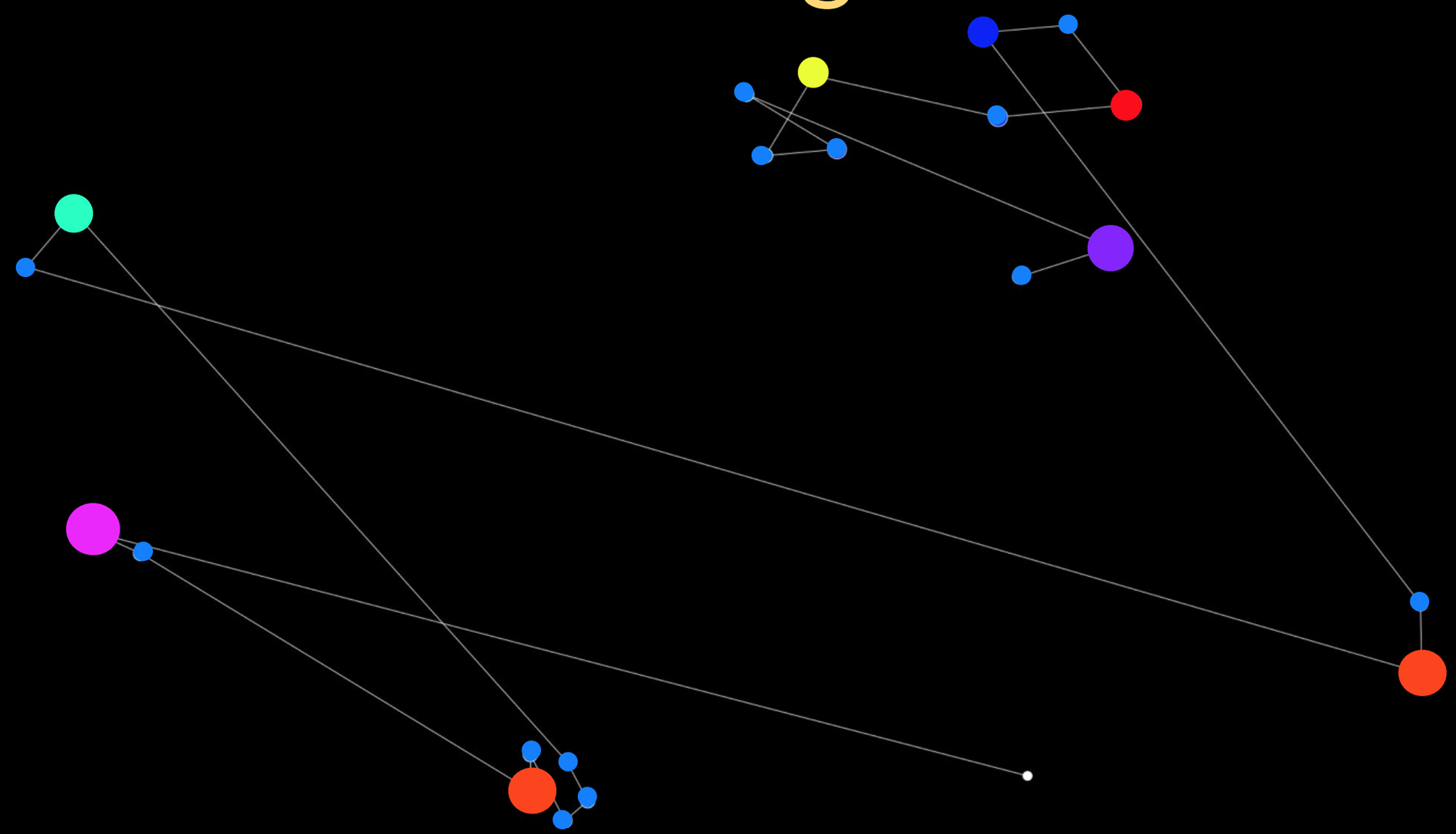


Below = Data Use Data



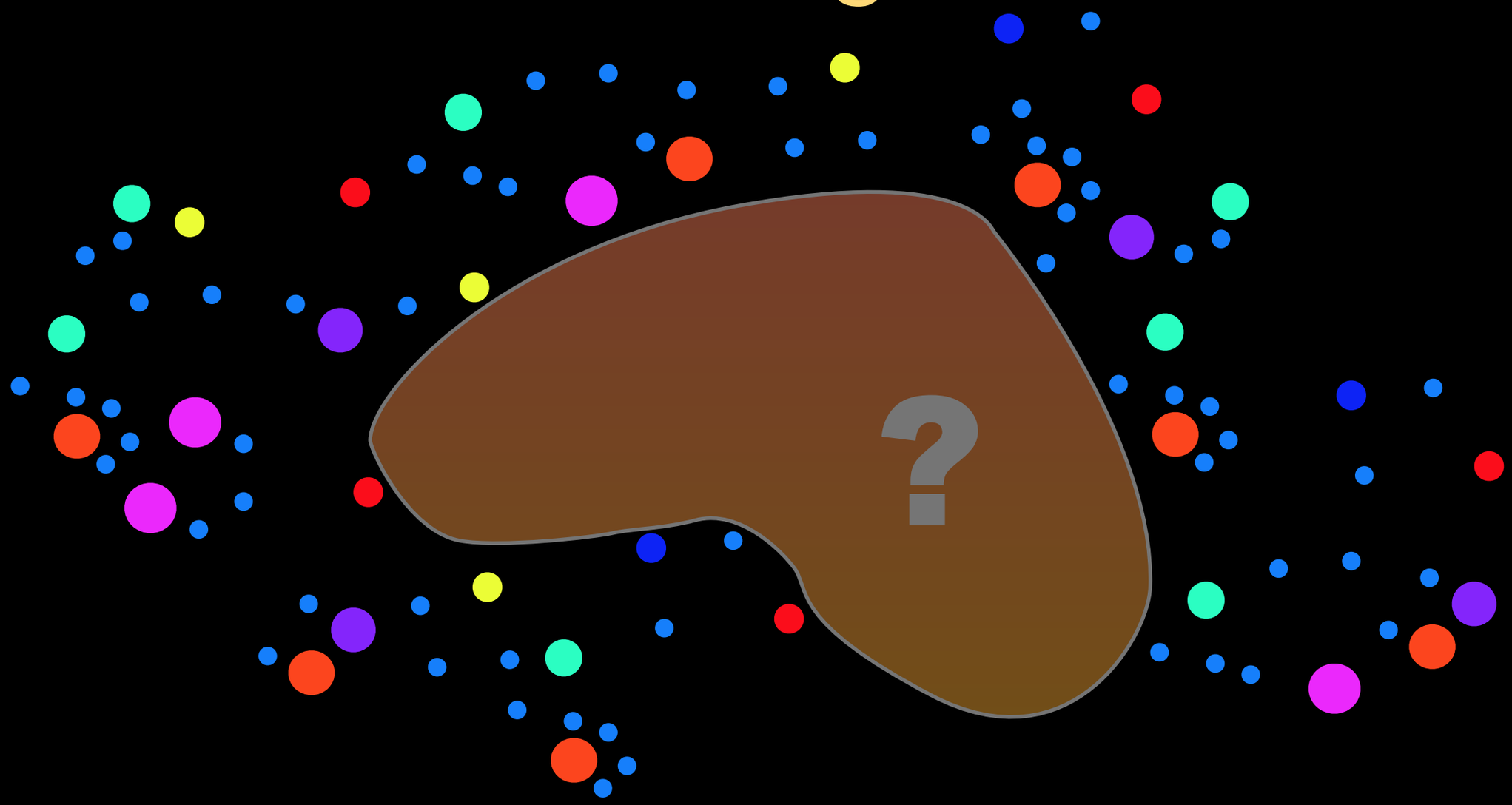
"Data Use Data"
could be used for...

...finding opportunities in scientific "terra incognita"...

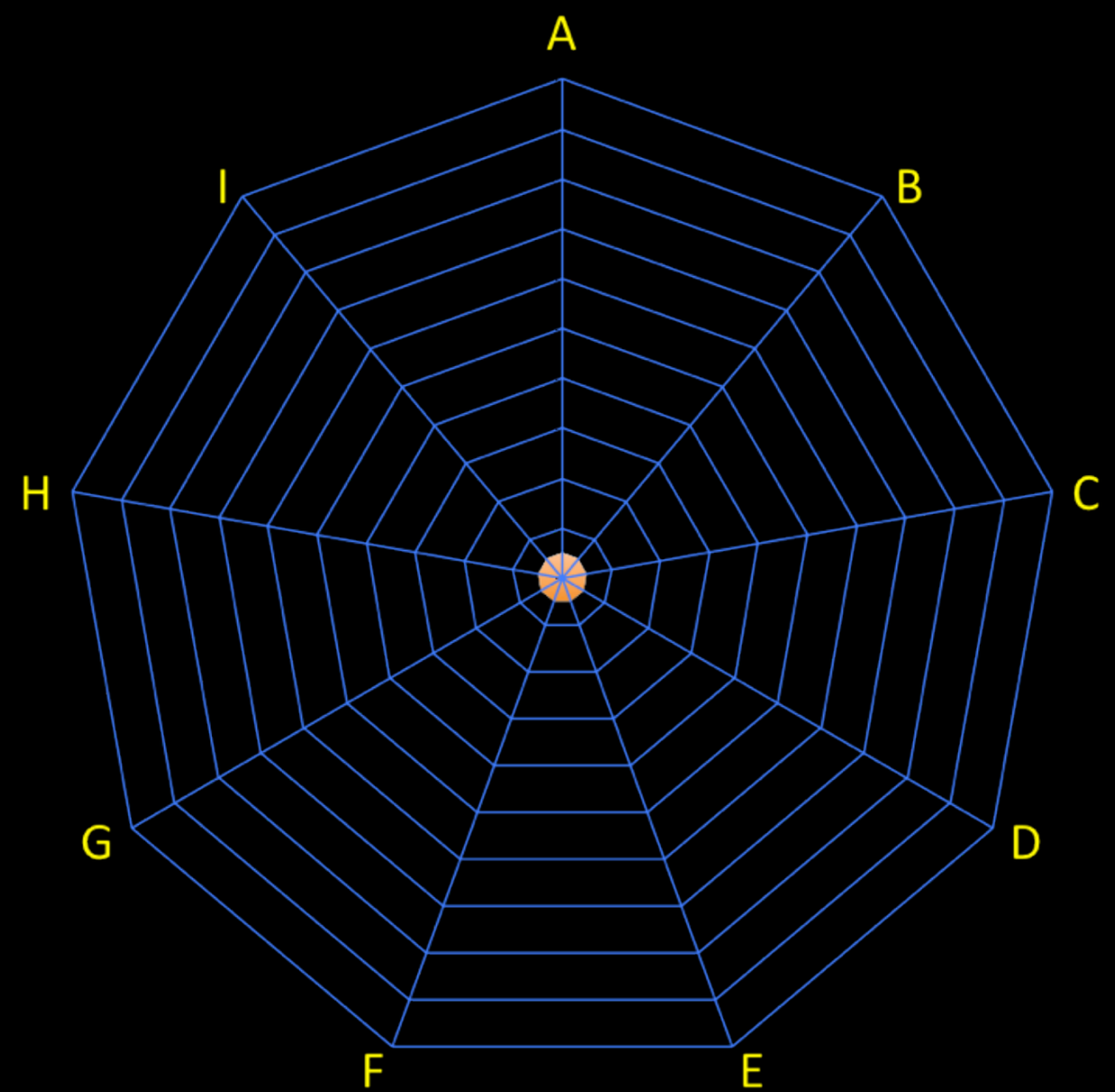


...finding opportunities in scientific "terra incognita"...

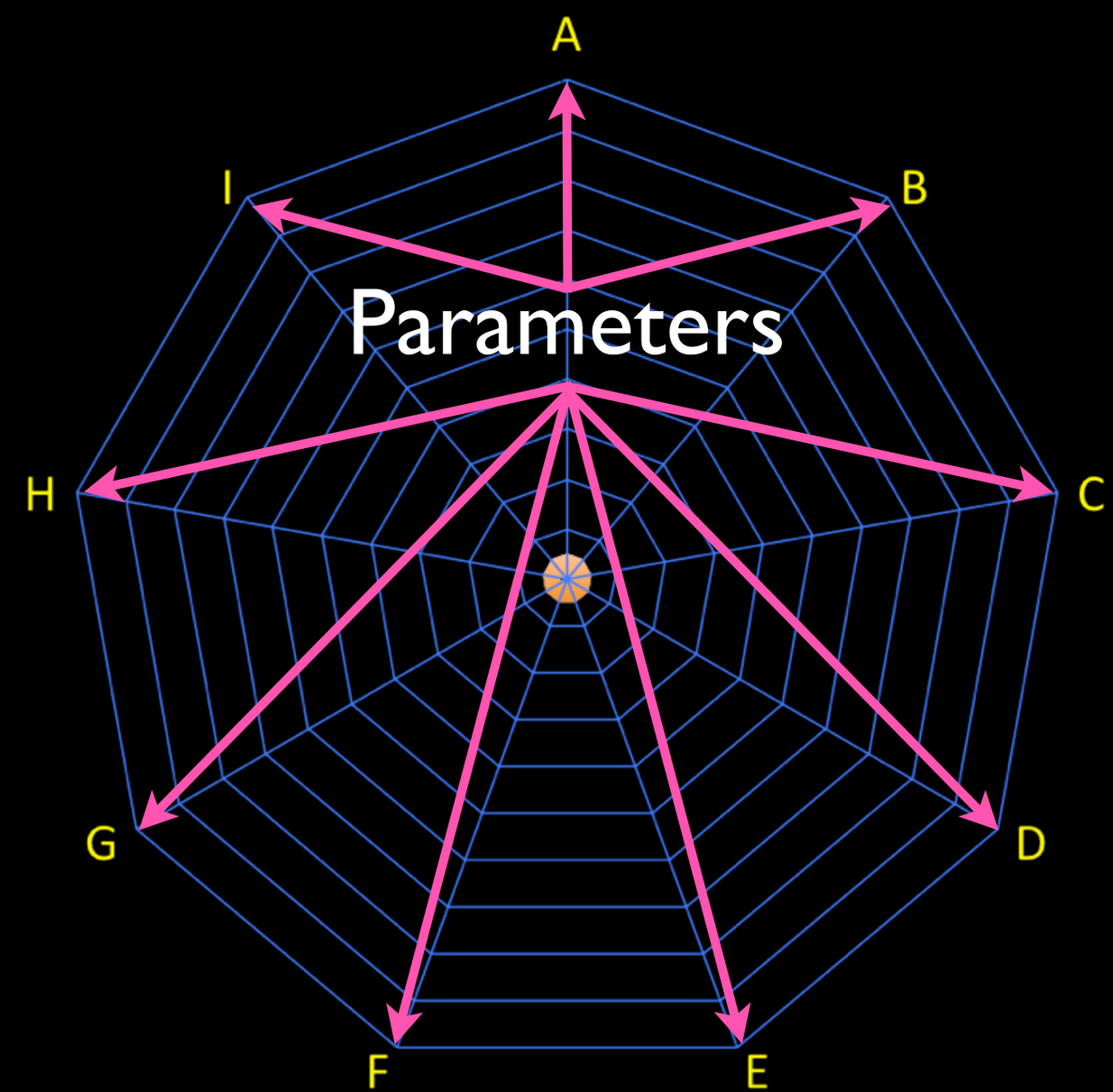
...finding opportunities in scientific "terra incognita"...



...finding potential collaborators...

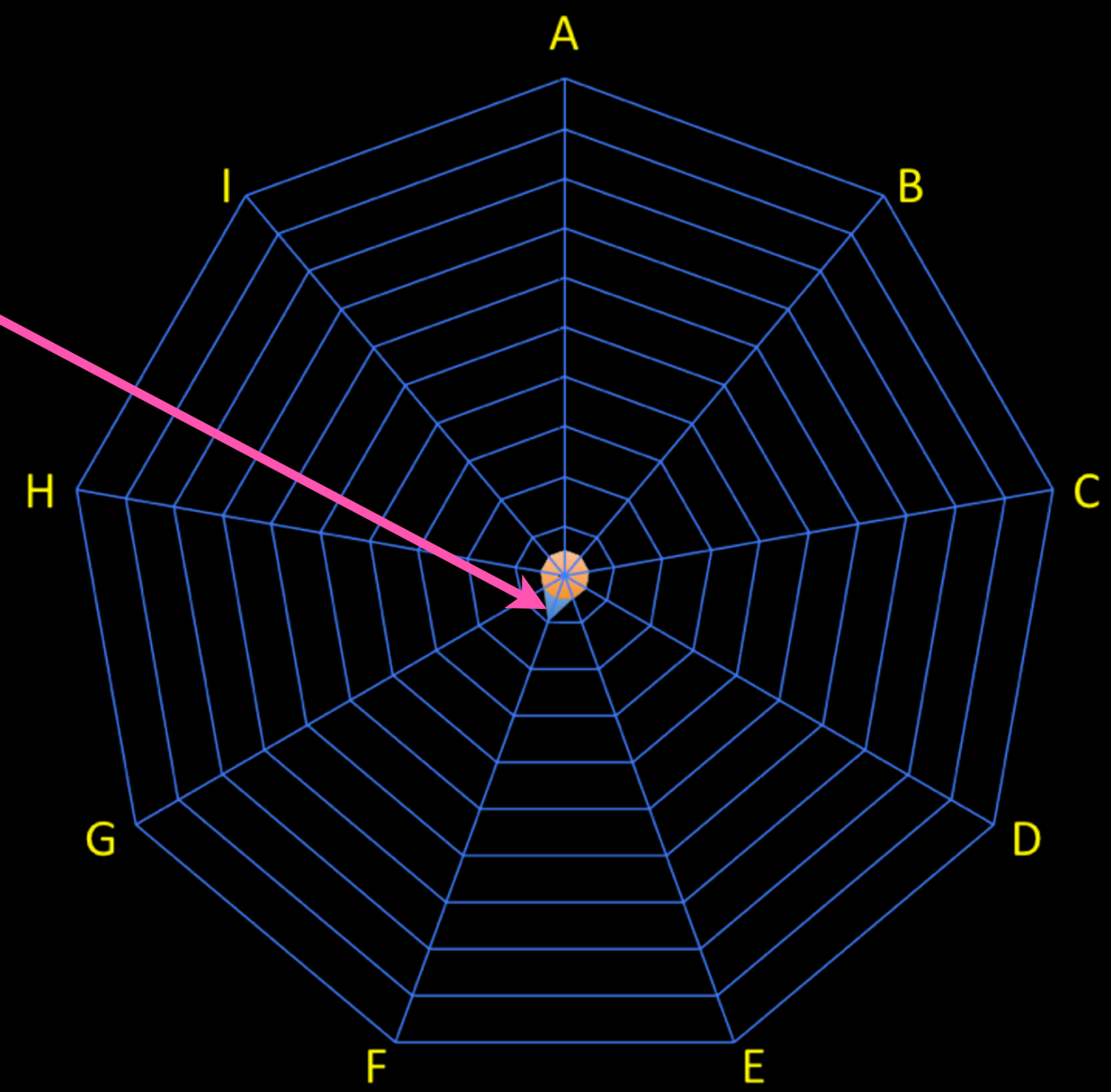


...finding potential collaborators...

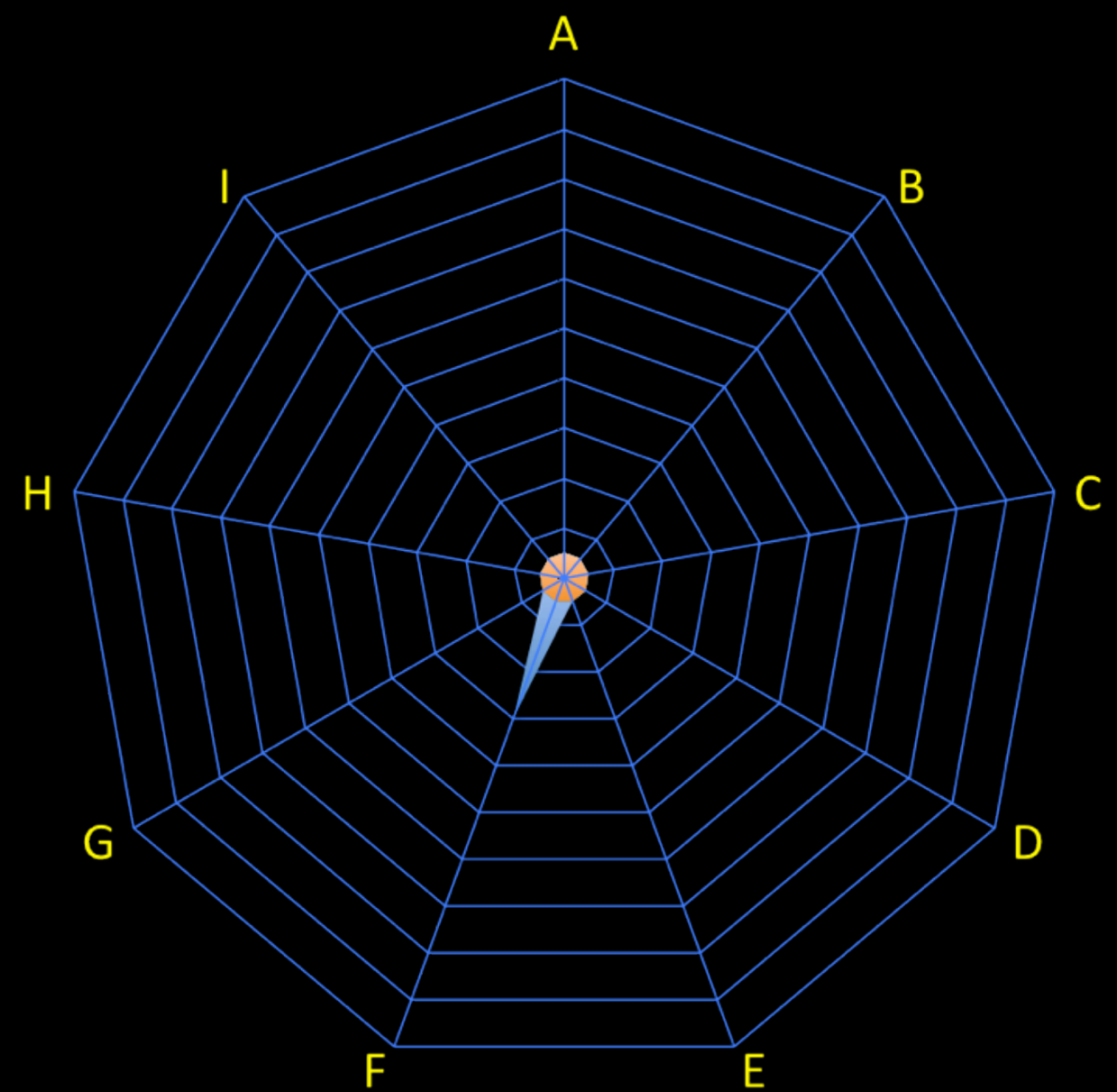


...finding potential collaborators...

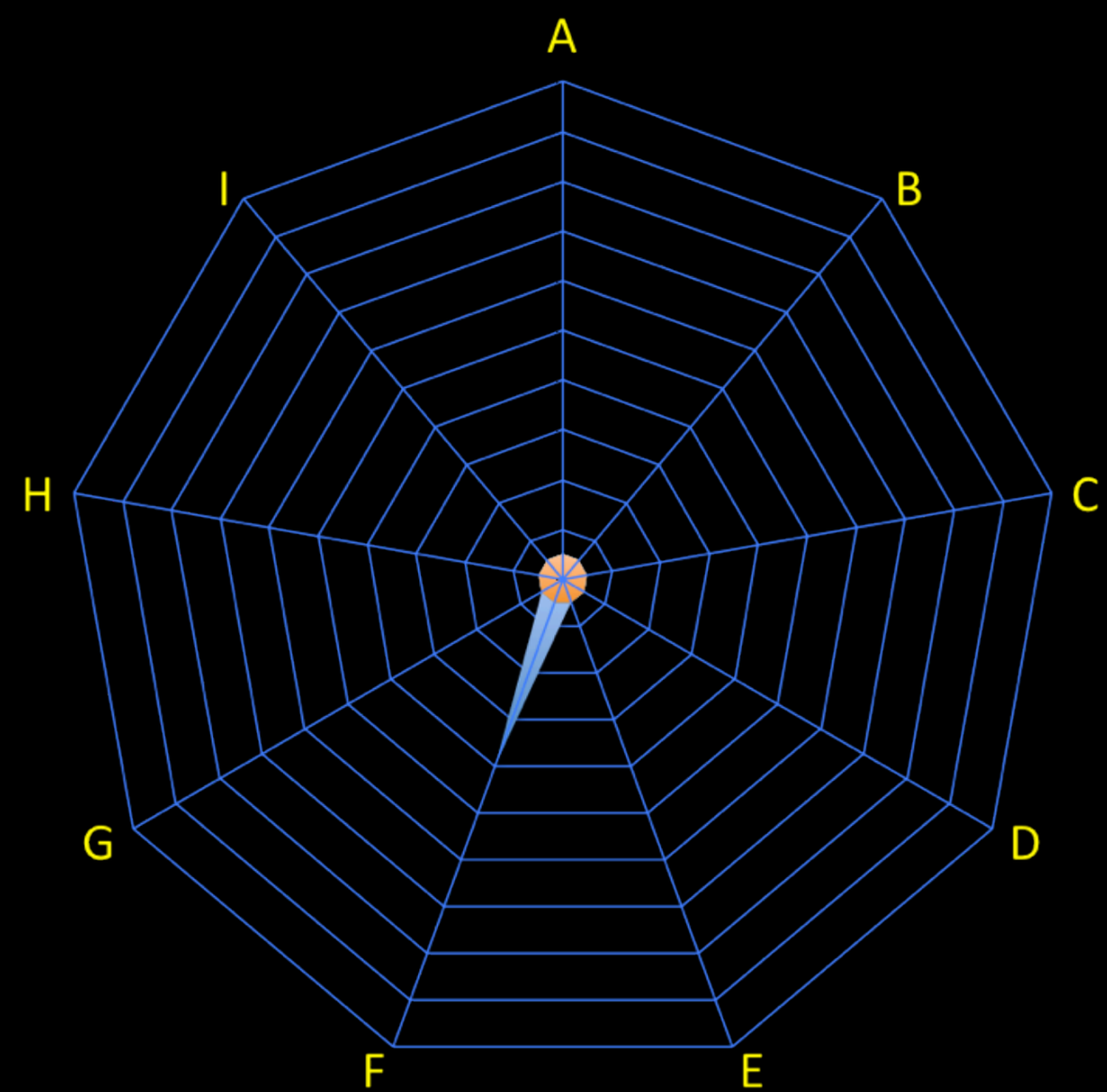
Tried a new value for parameter F



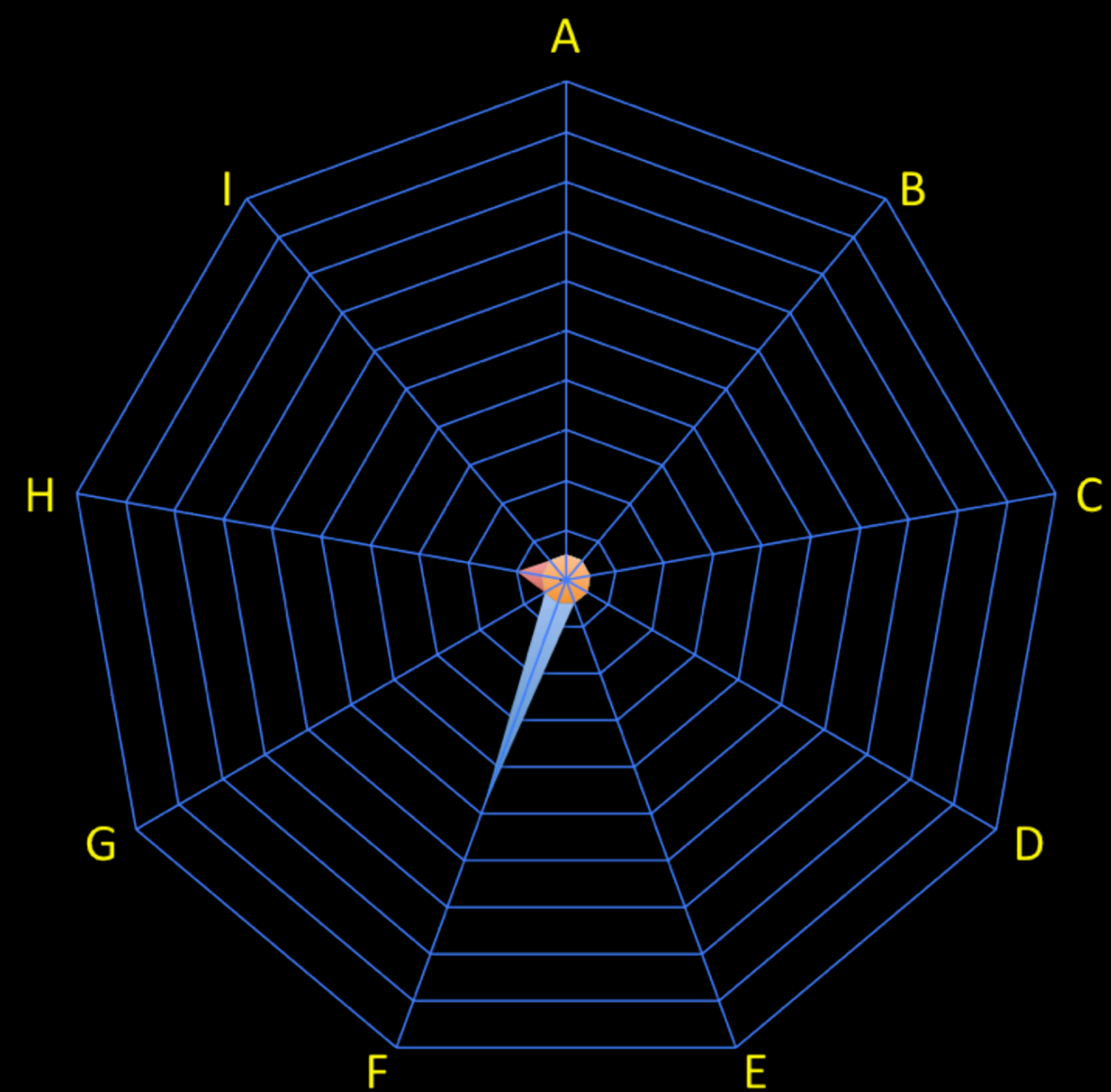
...finding potential collaborators...



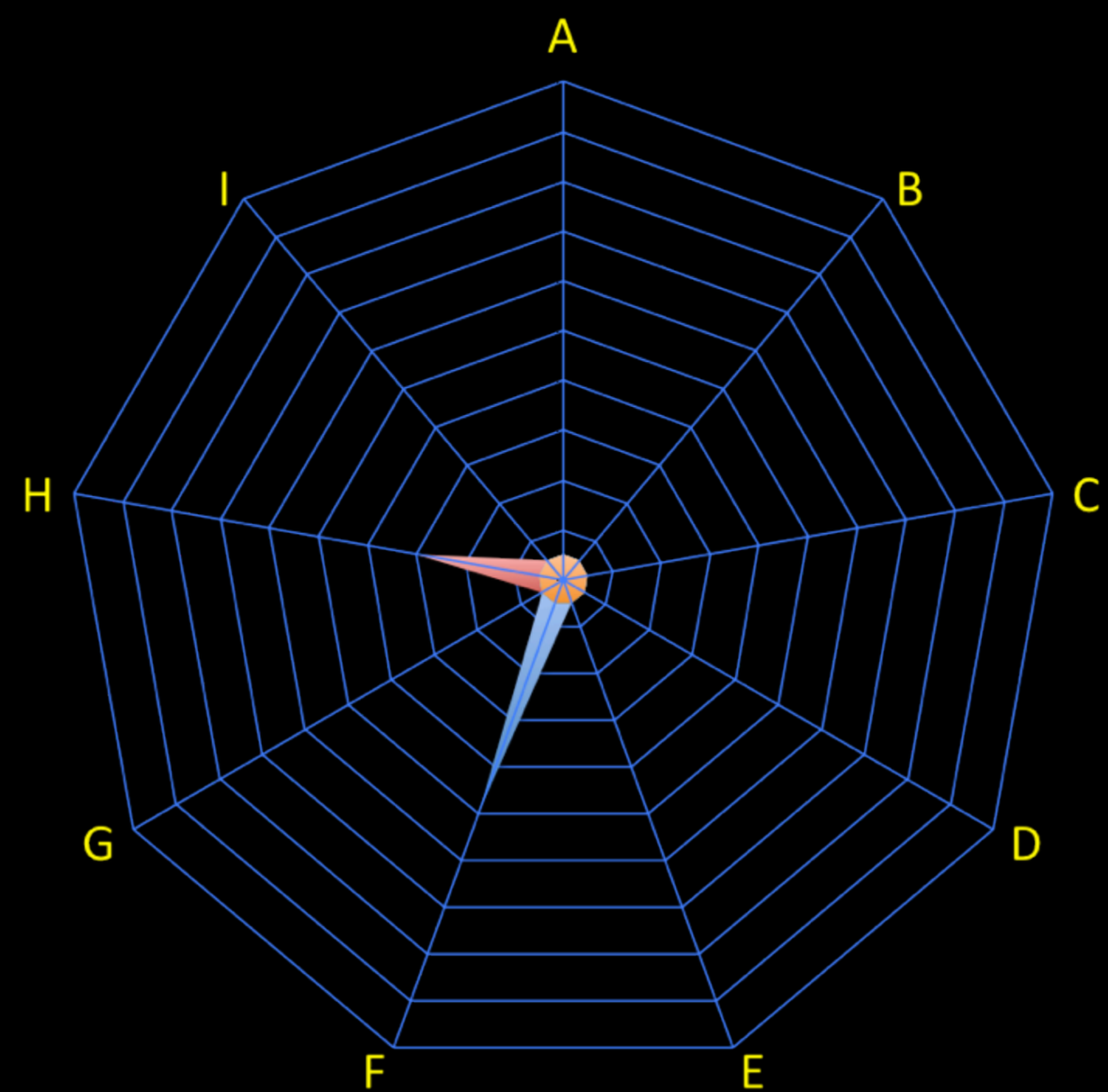
...finding potential collaborators...



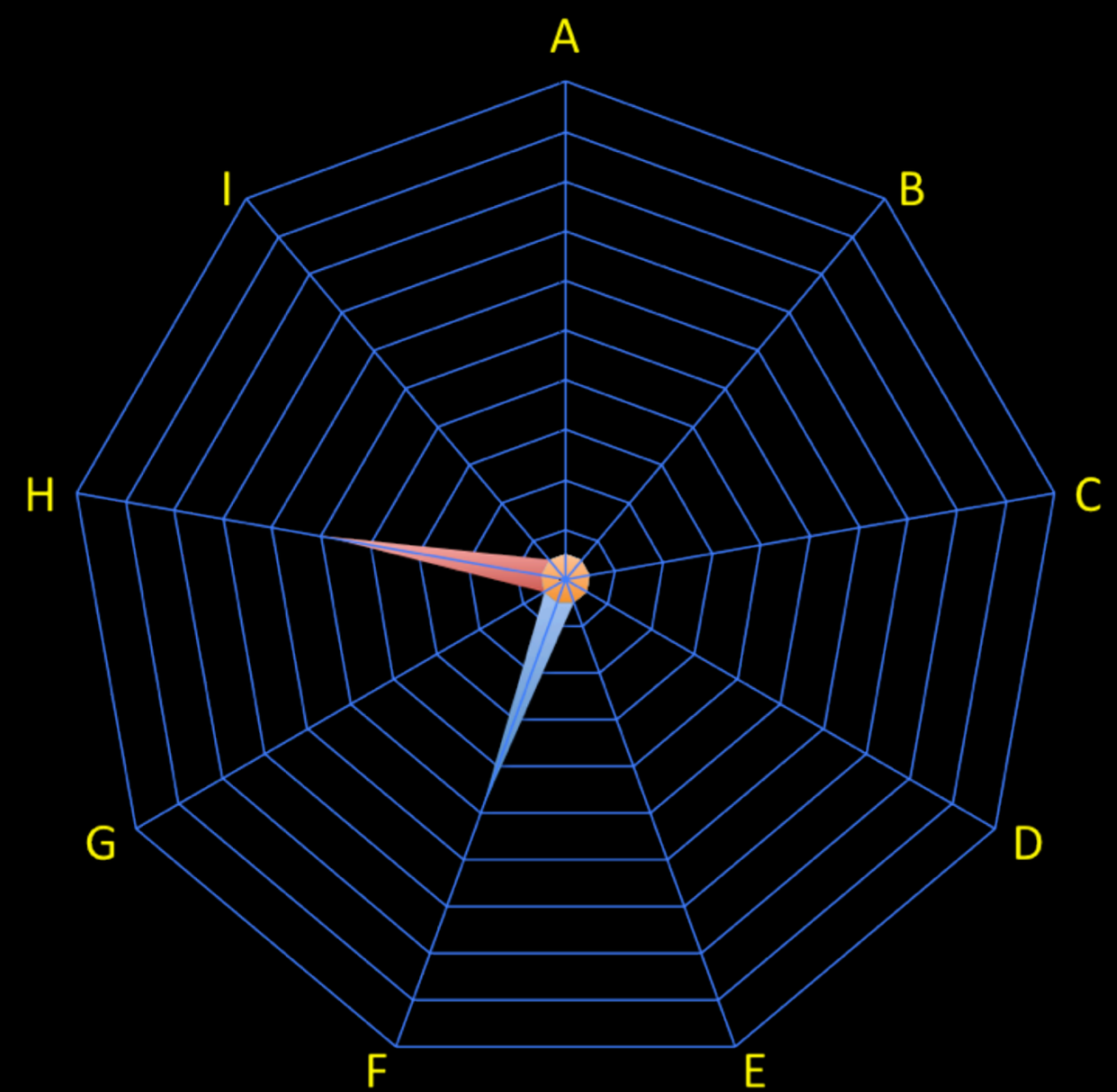
...finding potential collaborators...



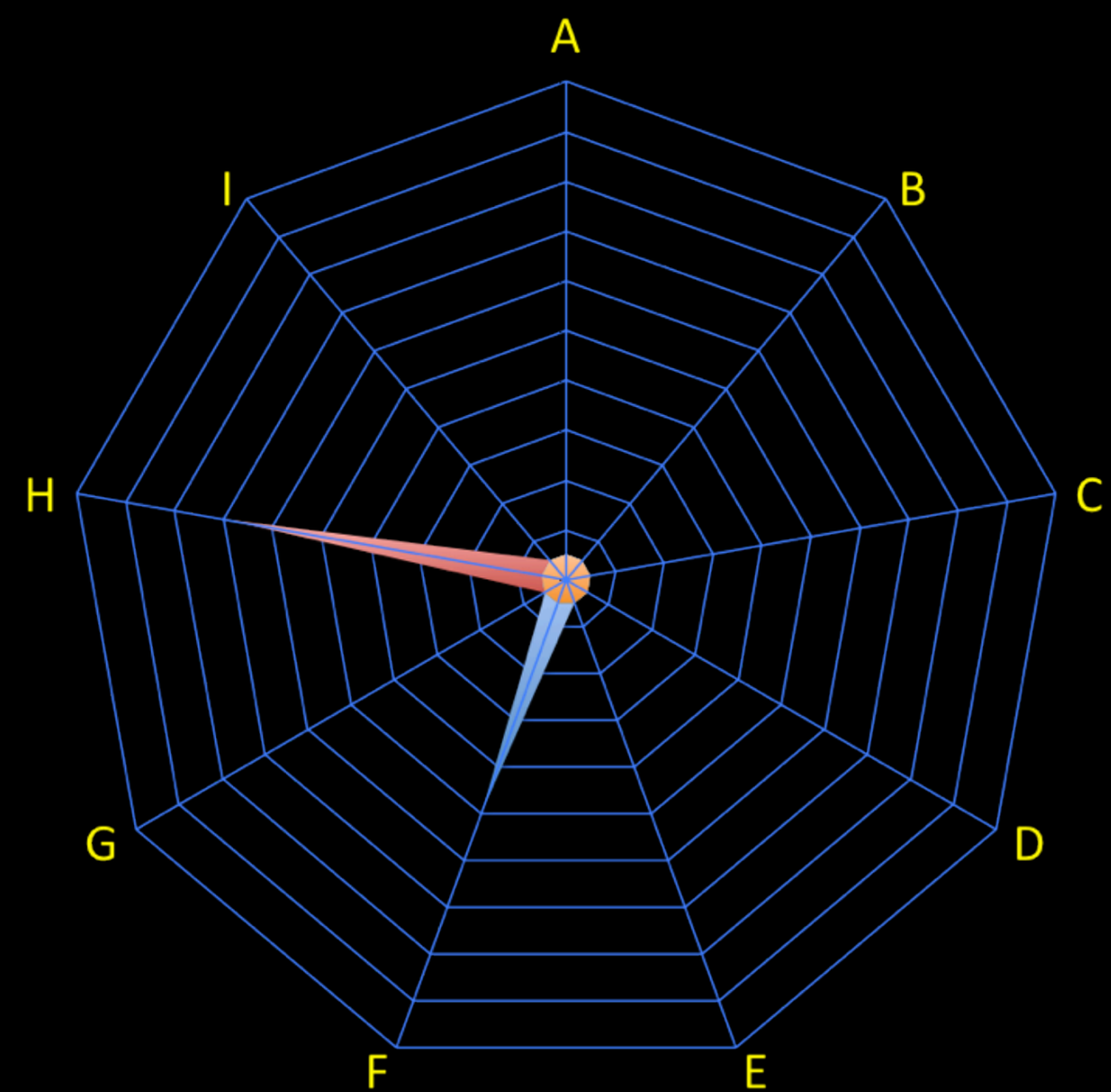
...finding potential collaborators...



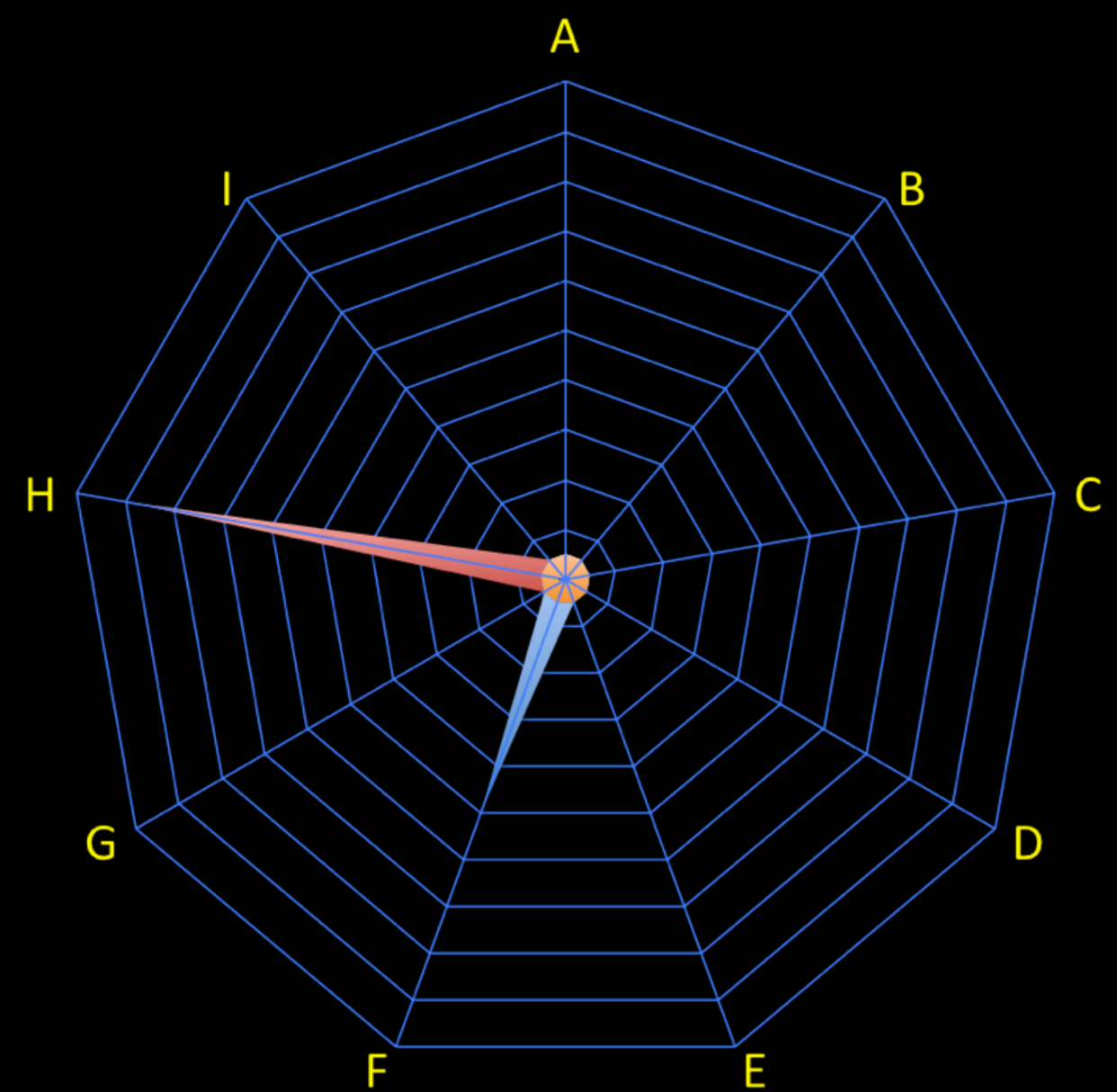
...finding potential collaborators...



...finding potential collaborators...

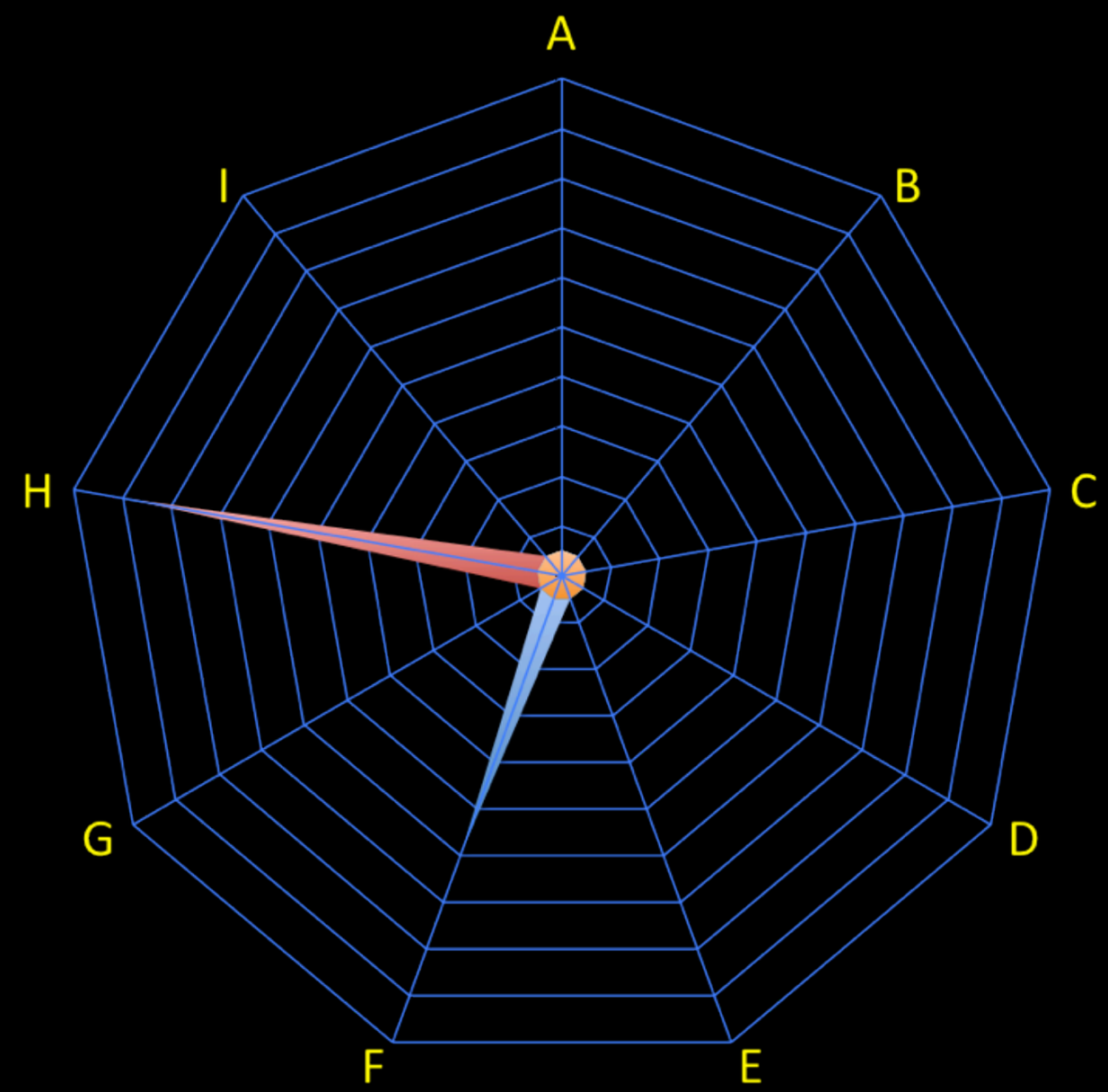


...finding potential collaborators...

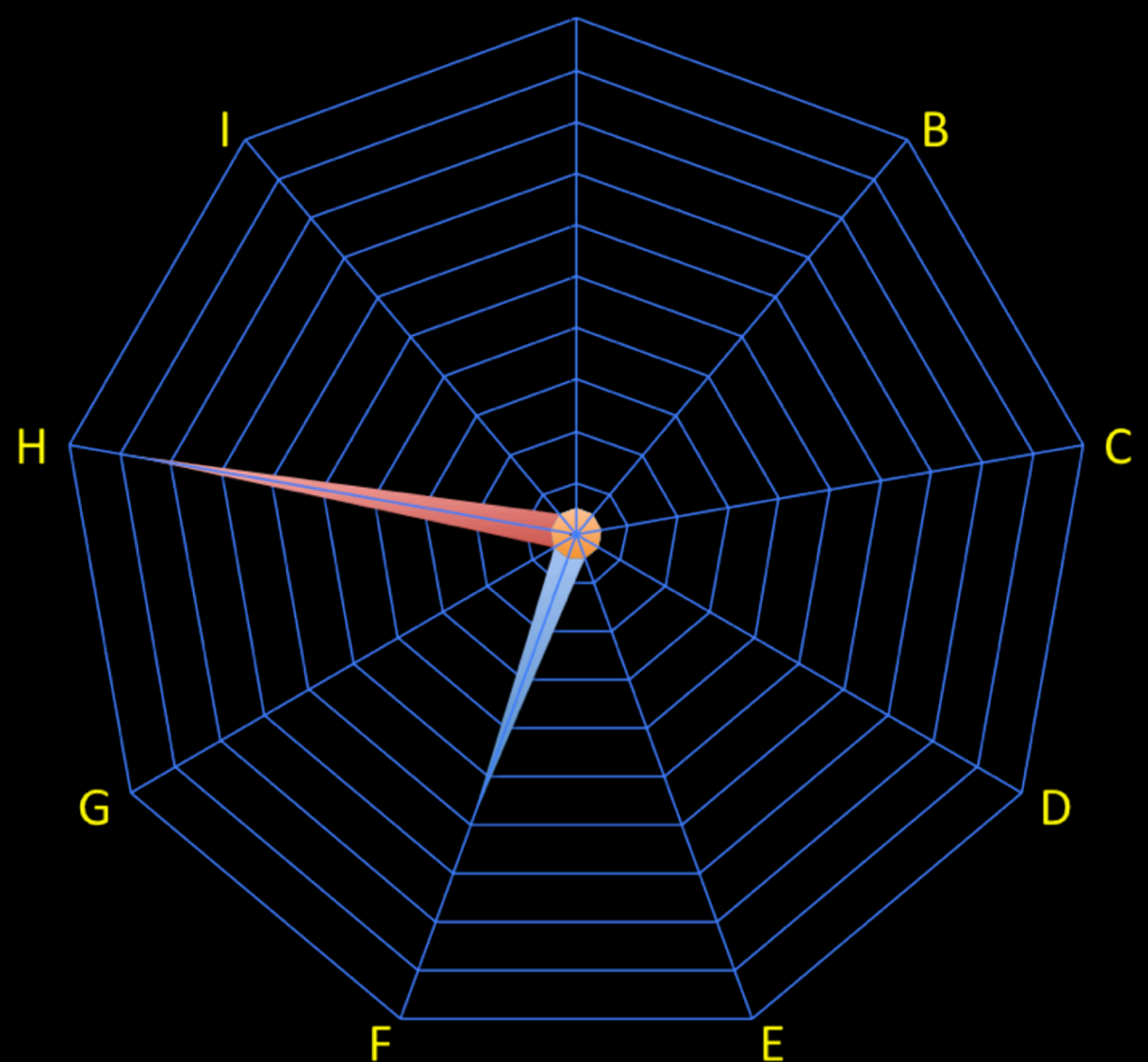


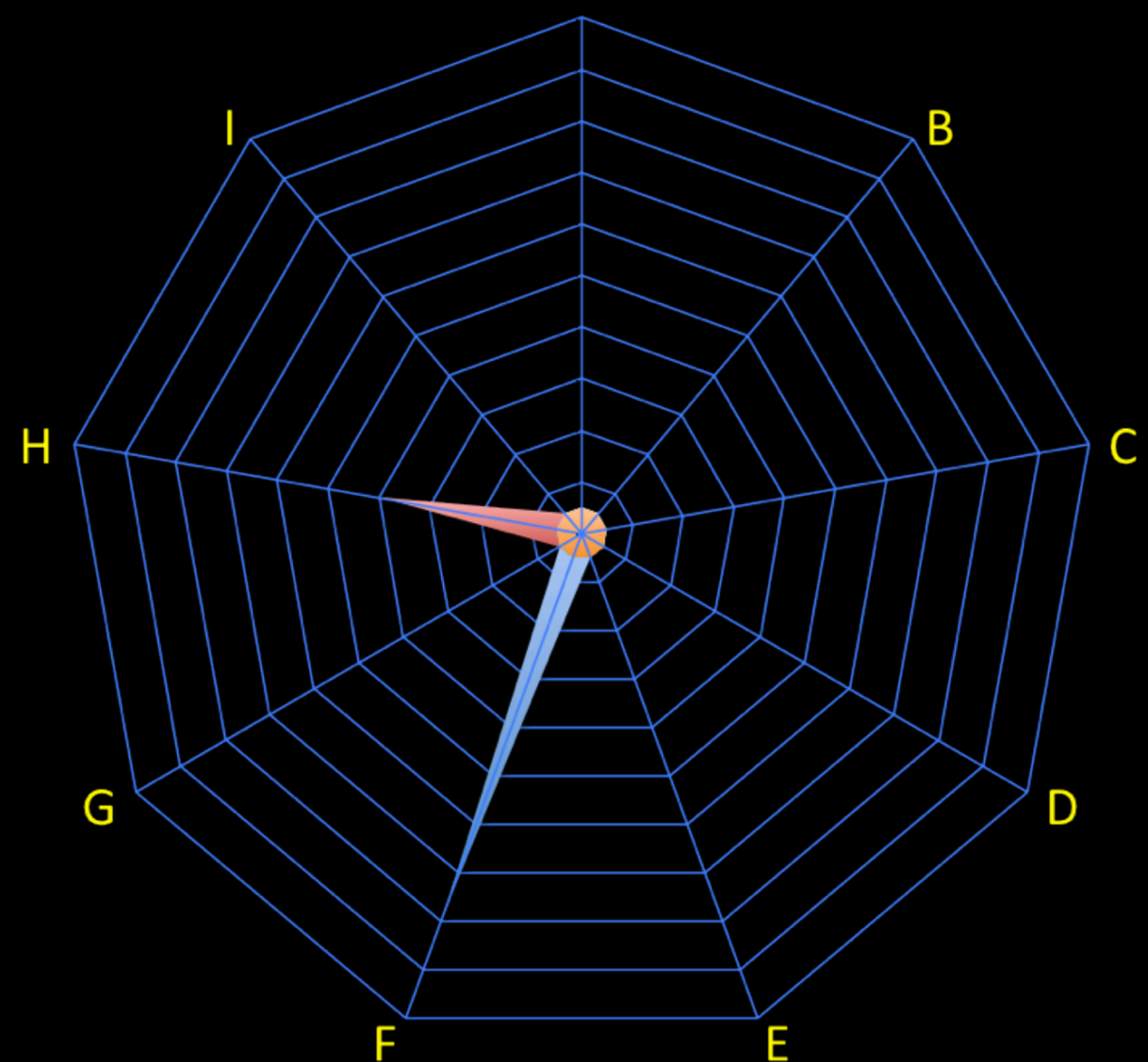
...finding potential collaborators...

One user who has tried various combinations of parameters F and H

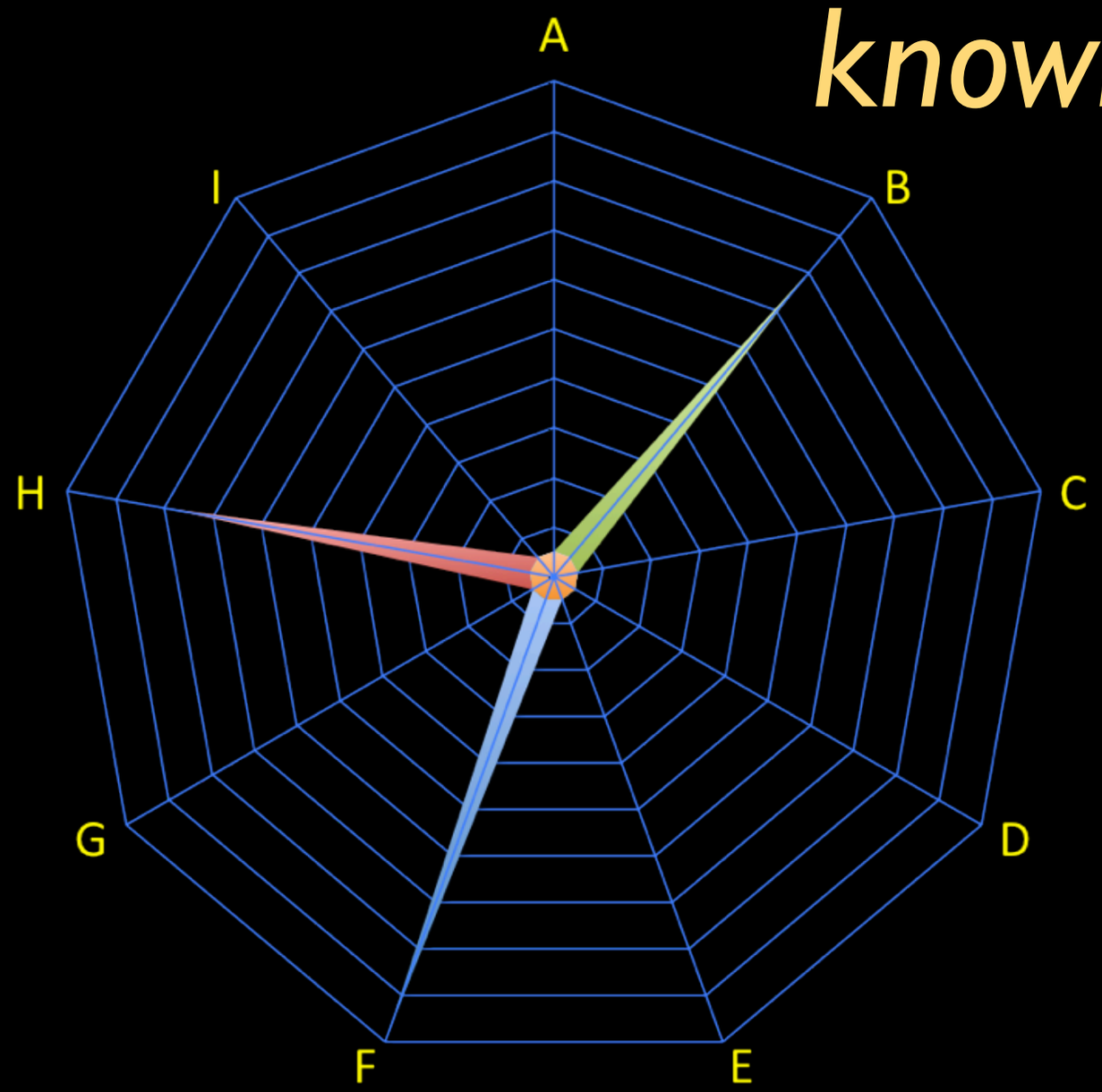


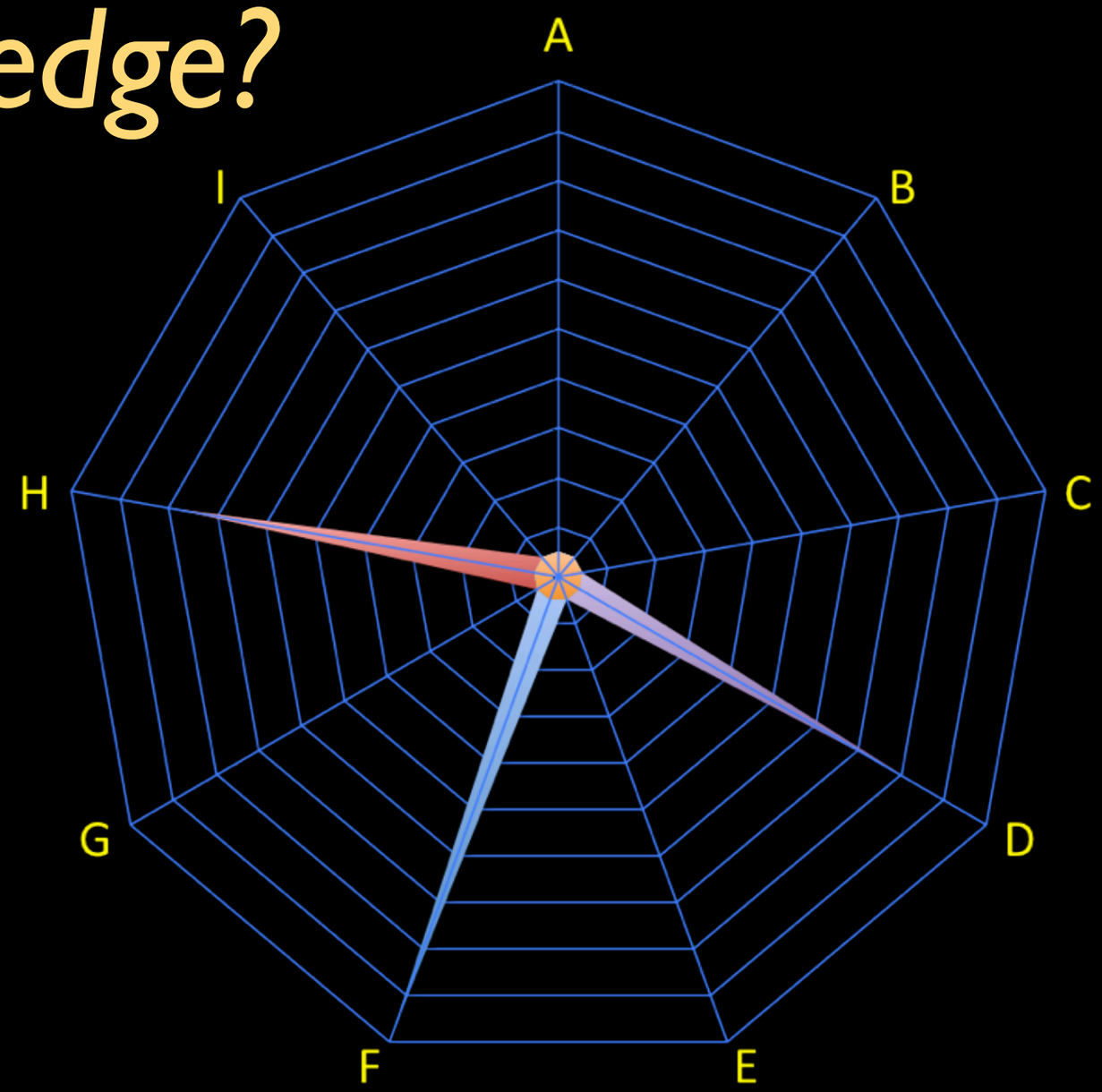
...finding potential collaborators... Should these two share knowledge?





...finding potential collaborators... Do these two have complementary knowledge?





It is likely that

data about how data are used

will be larger in scale than the data themselves.